Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1N4S
Title	:	Protein Geranylgeranyltransferase type-I Complexed with GGPP and a Geranylgeranylated KKKSKTKCVIL Peptide Product
Authors	:	Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on	:	2002-11-01
Resolution	:	2.60 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 ⓘ symbol.

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

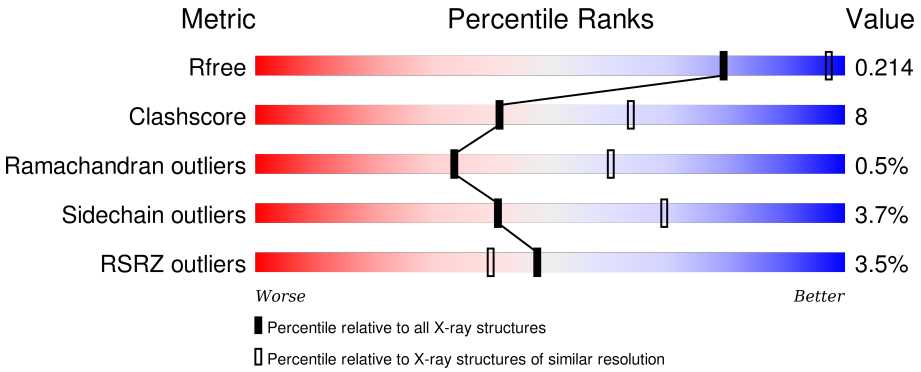
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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% 68% 14% • 17%
1	C	377	2% 67% 16% • 17%
1	E	377	3% 63% 19% • 17%
1	G	377	2% 66% 16% • 17%
1	I	377	2% 68% 15% • 17%

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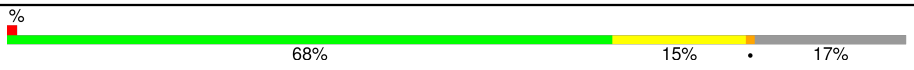
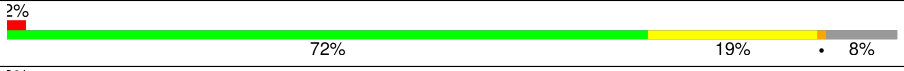
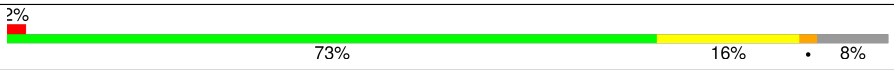
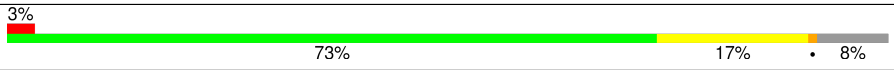
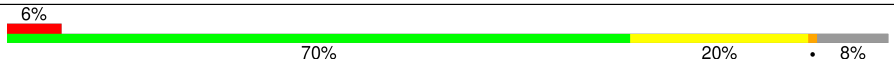
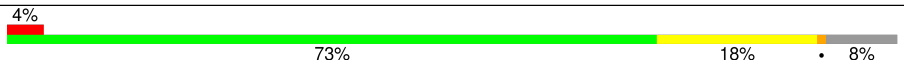
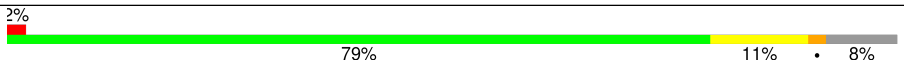
Mol	Chain	Length	Quality of chain
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

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	1402	-	-	-	X
5	CL	G	1405	-	-	-	X
7	GER	M	1108	-	-	-	X
7	GER	N	1208	-	-	-	X
7	GER	O	1308	-	-	-	X
7	GER	P	1408	-	-	-	X
7	GER	Q	1508	-	-	-	X
7	GER	R	1608	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33924 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			
3	O	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	P	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	Q	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	R	5	Total	C	N	O	S	0	0	0
			39	26	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	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		

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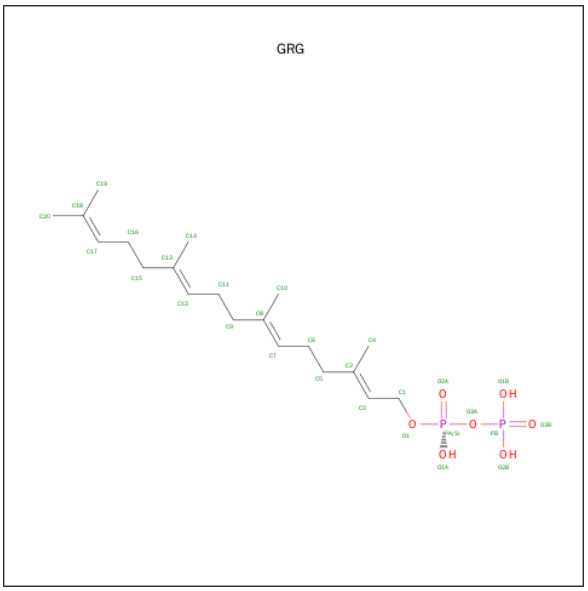
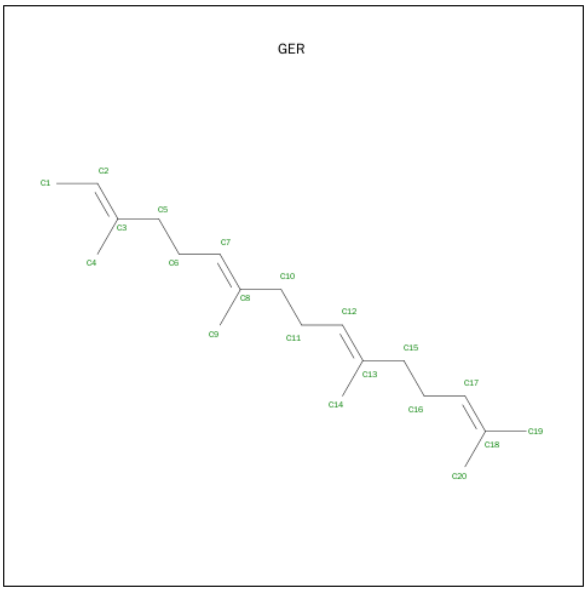
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0

- 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 29 20 7 2	0	0
6	D	1	Total C O P 29 20 7 2	0	0
6	F	1	Total C O P 29 20 7 2	0	0
6	H	1	Total C O P 29 20 7 2	0	0
6	J	1	Total C O P 29 20 7 2	0	0
6	L	1	Total C O P 29 20 7 2	0	0

- 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
7	O	1	Total C 20 20	0	0
7	P	1	Total C 20 20	0	0
7	Q	1	Total C 20 20	0	0
7	R	1	Total C 20 20	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	89	Total O 89 89	0	0
8	B	79	Total O 79 79	0	0
8	C	93	Total O 93 93	0	0
8	D	121	Total O 121 121	0	0
8	E	85	Total O 85 85	0	0
8	F	100	Total O 100 100	0	0

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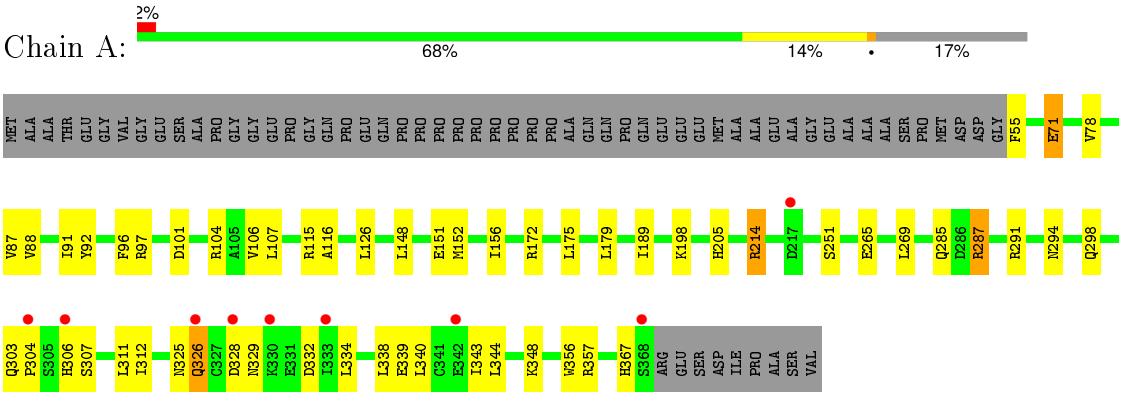
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	86	Total O 86 86	0	0
8	H	56	Total O 56 56	0	0
8	I	121	Total O 121 121	0	0
8	J	88	Total O 88 88	0	0
8	K	211	Total O 211 211	0	0
8	L	157	Total O 157 157	0	0
8	M	2	Total O 2 2	0	0
8	N	2	Total O 2 2	0	0
8	O	1	Total O 1 1	0	0
8	P	1	Total O 1 1	0	0
8	Q	1	Total O 1 1	0	0
8	R	3	Total O 3 3	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.

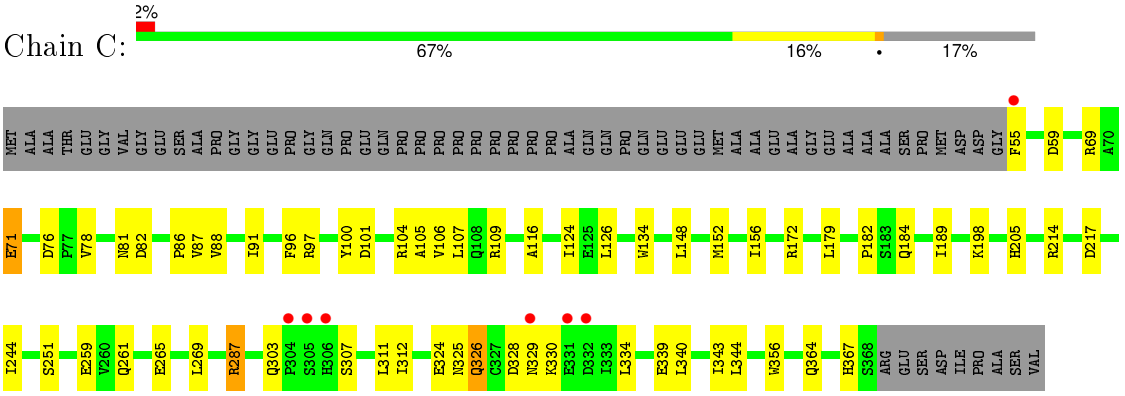
- Molecule 1: protein farnesyltransferase alpha subunit

Chain A:



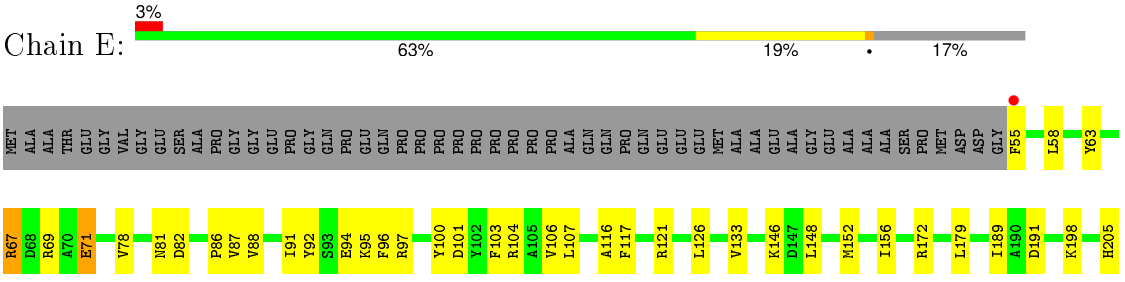
- Molecule 1: protein farnesyltransferase alpha subunit

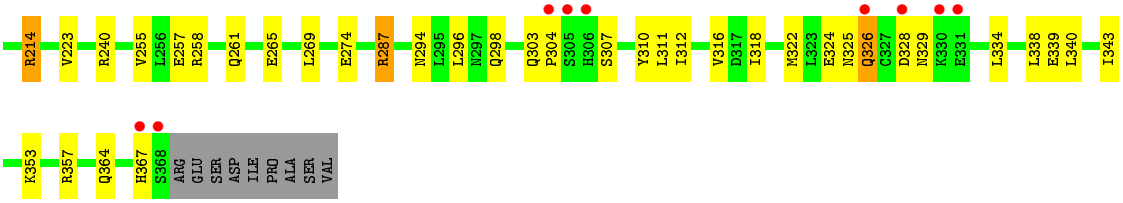
Chain C:



- Molecule 1: protein farnesyltransferase alpha subunit

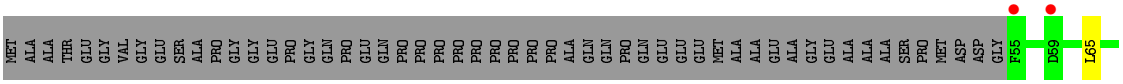
Chain E:

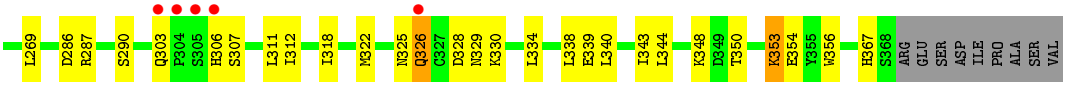




• Molecule 1: protein farnesyltransferase alpha subunit

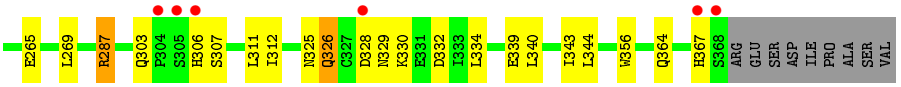
Chain G:





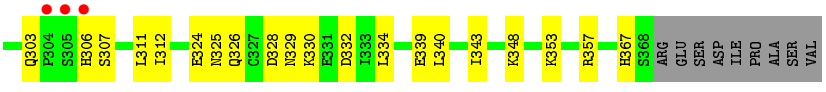
• Molecule 1: protein farnesyltransferase alpha subunit

Chain I:



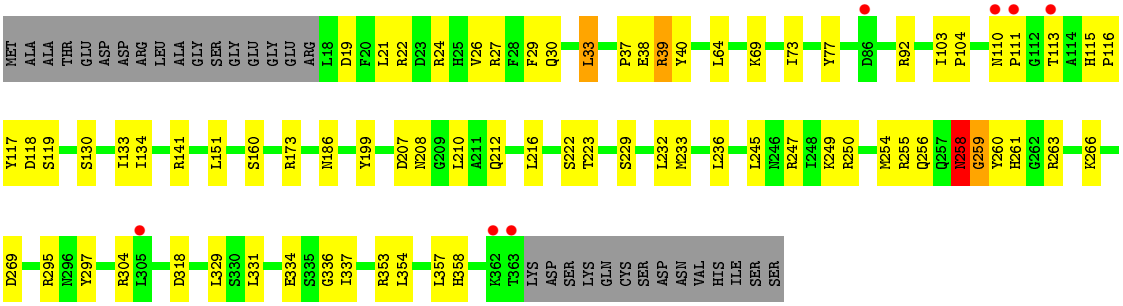
• Molecule 1: protein farnesyltransferase alpha subunit

Chain K:



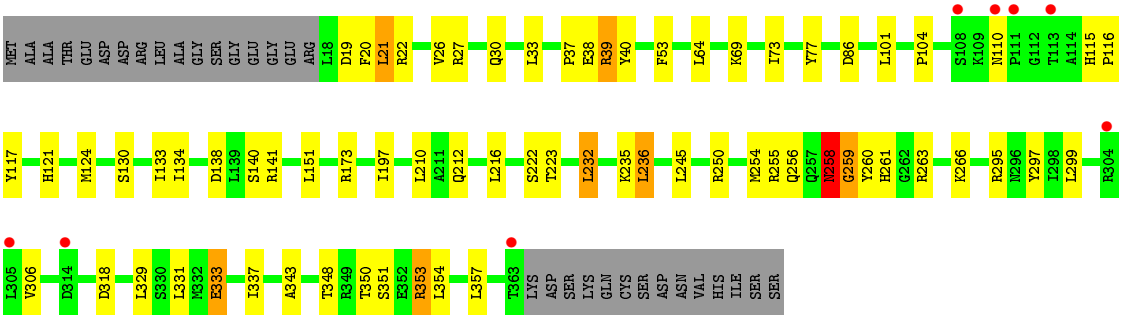
• Molecule 2: geranyltransferase type-I beta subunit

Chain B:



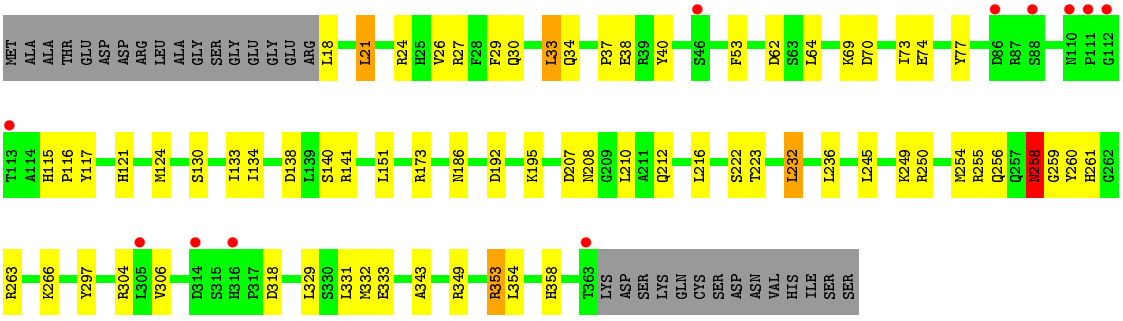
• Molecule 2: geranyltransferase type-I beta subunit

Chain D:



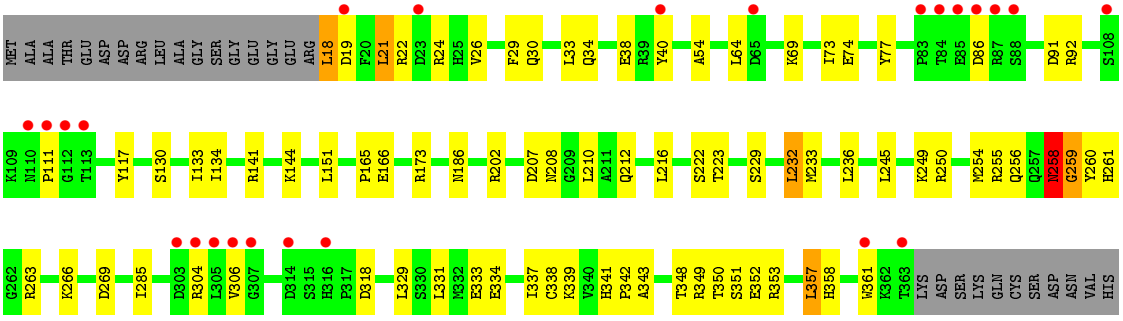
• Molecule 2: geranyltransferase type-I beta subunit

Chain F:



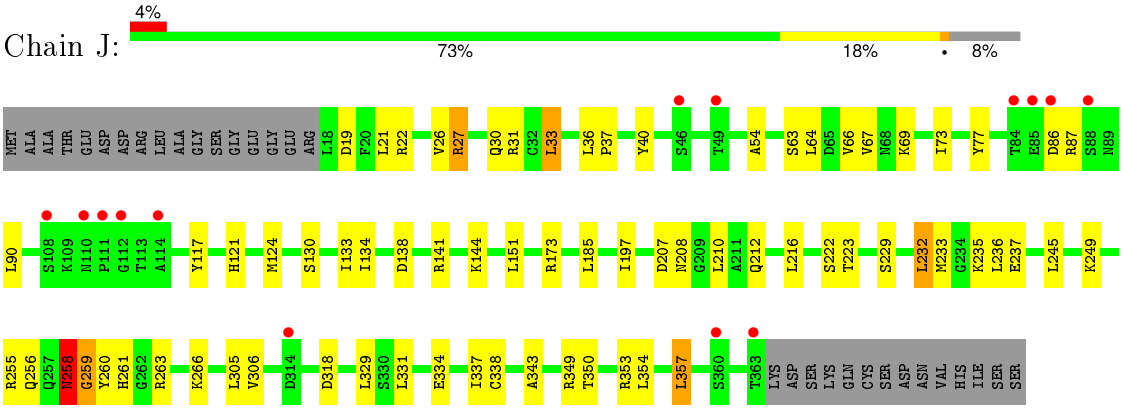
• Molecule 2: geranyltransferase type-I beta subunit

Chain H:



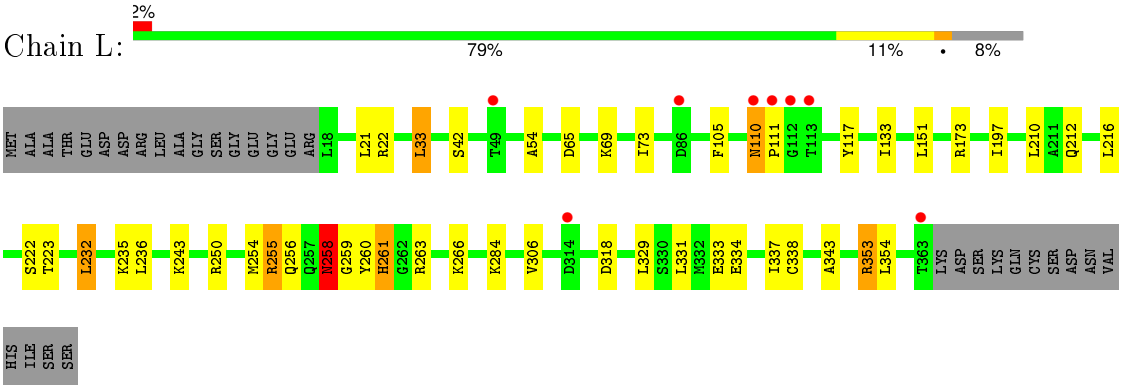
• Molecule 2: geranyltransferase type-I beta subunit

Chain J:



• Molecule 2: geranyltransferase type-I beta subunit

Chain L:

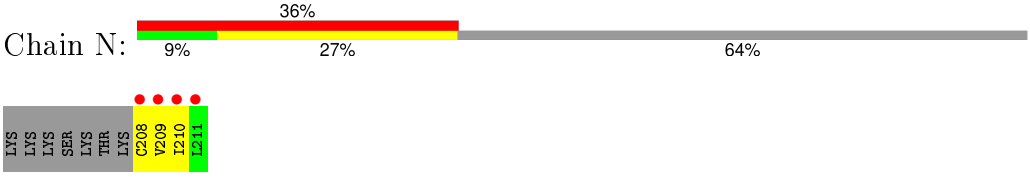


• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain M:

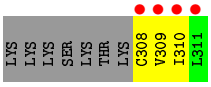
• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain N:

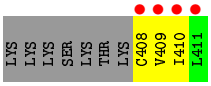


• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain O:



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



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

• 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	271.12Å 268.43Å 184.82Å 90.00° 131.58° 90.00°	Depositor
Resolution (Å)	29.98 – 2.60 39.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.98-2.60) 99.7 (39.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.214 0.195 , 0.214	Depositor DCC
R_{free} test set	14968 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
Estimated twinning fraction	0.078 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 300409 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33924	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 2.25% 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	0.33	0/2695	0.51	0/3668
1	C	0.35	0/2709	0.52	0/3684
1	E	0.34	0/2708	0.53	0/3684
1	G	0.35	0/2699	0.52	0/3672
1	I	0.35	0/2722	0.52	0/3700
1	K	0.39	0/2737	0.55	0/3717
2	B	0.35	0/2759	0.59	2/3733 (0.1%)
2	D	0.37	0/2775	0.59	2/3752 (0.1%)
2	F	0.37	0/2780	0.59	2/3758 (0.1%)
2	H	0.34	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	0.62	0/29	0.88	0/37
3	N	0.57	0/29	0.91	0/37
3	O	0.60	0/29	0.91	0/37
3	P	0.56	0/29	0.89	0/37
3	Q	0.60	0/29	0.93	0/37
3	R	0.52	0/38	0.84	0/48
All	All	0.36	0/33081	0.56	12/44844 (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	D	0	1
2	F	0	1
All	All	0	3

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	F	259	GLY	N-CA-C	-5.86	98.46	113.10
2	H	259	GLY	N-CA-C	-5.83	98.53	113.10
2	D	259	GLY	N-CA-C	-5.83	98.53	113.10
2	J	259	GLY	N-CA-C	-5.81	98.57	113.10
2	L	259	GLY	N-CA-C	-5.71	98.83	113.10
2	J	258	ASN	N-CA-C	-5.67	95.70	111.00
2	B	259	GLY	N-CA-C	-5.54	99.26	113.10
2	B	258	ASN	N-CA-C	-5.50	96.14	111.00
2	F	258	ASN	N-CA-C	-5.39	96.44	111.00
2	D	258	ASN	N-CA-C	-5.39	96.45	111.00
2	H	258	ASN	N-CA-C	-5.33	96.60	111.00
2	L	258	ASN	N-CA-C	-5.33	96.59	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	D	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	43	0
1	C	2643	0	2540	39	0
1	E	2642	0	2534	52	0
1	G	2633	0	2524	52	0
1	I	2656	0	2560	35	0
1	K	2671	0	2588	38	0
2	B	2697	0	2600	51	0
2	D	2713	0	2628	51	0
2	F	2718	0	2635	38	0
2	H	2694	0	2590	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2711	0	2616	47	0
2	L	2723	0	2643	27	0
3	M	30	0	34	4	0
3	N	30	0	34	3	0
3	O	30	0	34	4	0
3	P	30	0	34	5	0
3	Q	30	0	34	3	0
3	R	39	0	47	8	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	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	2	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	2	0
7	M	20	0	33	5	0
7	N	20	0	33	6	0
7	O	20	0	33	7	0
7	P	20	0	33	6	0
7	Q	20	0	33	4	0
7	R	20	0	33	6	0
8	A	89	0	0	1	0
8	B	79	0	0	2	0
8	C	93	0	0	1	0
8	D	121	0	0	2	0
8	E	85	0	0	0	0
8	F	100	0	0	3	0
8	G	86	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	56	0	0	4	0
8	I	121	0	0	1	1
8	J	88	0	0	2	0
8	K	211	0	0	4	0
8	L	157	0	0	2	0
8	M	2	0	0	0	0
8	N	2	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	3	0	0	2	0
All	All	33924	0	31591	545	1

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

All (545) 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:K:156:ILE:HG12	1:K:172:ARG:HH12	1.01	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.12	1.10
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.11	1.07
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.06	1.06
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.18	1.04
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.24	1.03
2:L:212:GLN:HE21	2:L:222:SER:HB3	1.21	1.02
2:J:212:GLN:NE2	2:J:222:SER:HB3	1.82	0.94
2:J:212:GLN:HE21	2:J:222:SER:HB3	1.31	0.94
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.85	0.92
2:H:18:LEU:HA	2:H:304:ARG:NH2	1.84	0.92
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.52	0.90
5:G:1405:CL:CL	8:G:1411:HOH:O	2.28	0.89
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.39	0.86
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.91	0.84
2:D:39:ARG:H	2:D:39:ARG:HD2	1.42	0.83
1:A:152:MET:O	1:A:156:ILE:HG13	1.79	0.83
2:L:212:GLN:NE2	2:L:222:SER:HB3	1.95	0.81
2:B:173:ARG:HG2	6:B:1501:GRG:H112	1.62	0.81
2:L:42:SER:HG	3:R:607:LYS:N	1.79	0.81
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.63	0.81
2:L:173:ARG:HG2	6:L:1506:GRG:H112	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:MET:O	1:G:156:ILE:HG13	1.82	0.80
2:D:37:PRO:HB2	2:D:39:ARG:CD	2.12	0.79
2:J:173:ARG:HG2	6:J:1505:GRG:H112	1.64	0.79
1:K:152:MET:O	1:K:156:ILE:HG13	1.82	0.78
2:D:173:ARG:HG2	6:D:1502:GRG:H112	1.65	0.78
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.49	0.78
1:I:152:MET:O	1:I:156:ILE:HG13	1.83	0.78
1:E:152:MET:O	1:E:156:ILE:HG13	1.84	0.77
2:B:353:ARG:HD2	8:B:1566:HOH:O	1.83	0.77
2:F:173:ARG:HG2	6:F:1503:GRG:H112	1.65	0.77
1:E:214:ARG:O	1:E:214:ARG:HG3	1.85	0.76
1:C:152:MET:O	1:C:156:ILE:HG13	1.84	0.75
2:H:173:ARG:HG2	6:H:1504:GRG:H112	1.69	0.75
2:H:348:THR:O	2:H:352:GLU:HG2	1.88	0.74
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.02	0.74
2:H:229:SER:O	2:H:233:MET:HG3	1.86	0.74
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.70	0.73
5:K:1408:CL:CL	8:K:1417:HOH:O	2.43	0.73
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.04	0.73
2:F:212:GLN:NE2	2:F:222:SER:HB3	2.04	0.73
1:C:100:TYR:HB3	1:C:104:ARG:HH21	1.53	0.72
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.96	0.72
2:B:24:ARG:HD3	2:B:27:ARG:HH22	1.54	0.71
2:D:37:PRO:HB2	2:D:39:ARG:HD2	1.72	0.71
2:D:37:PRO:HB2	2:D:39:ARG:HD3	1.73	0.71
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.93	0.70
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.72	0.70
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.56	0.70
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.73	0.70
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.73	0.69
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.97	0.69
2:B:318:ASP:HB2	7:M:1108:GER:H71	1.75	0.68
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.58	0.68
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.75	0.68
2:H:144:LYS:HE2	8:H:1546:HOH:O	1.95	0.67
2:F:318:ASP:HB2	7:O:1308:GER:H71	1.76	0.67
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.75	0.67
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.95	0.67
1:I:91:ILE:HD12	1:I:91:ILE:O	1.94	0.67
1:E:156:ILE:CG1	1:E:172:ARG:HH12	2.01	0.67
2:H:212:GLN:NE2	2:H:222:SER:HB3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:LYS:O	2:D:73:ILE:HG13	1.94	0.66
2:J:318:ASP:HB2	7:Q:1508:GER:H71	1.77	0.66
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.26	0.66
1:G:91:ILE:HD12	1:G:91:ILE:O	1.96	0.66
2:L:338:CYS:HB3	8:L:1637:HOH:O	1.96	0.66
2:H:18:LEU:N	2:H:18:LEU:HD22	2.10	0.66
2:J:263:ARG:HG3	2:J:266:LYS:HG3	1.77	0.66
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.76	0.65
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.60	0.65
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.79	0.65
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.79	0.65
2:B:263:ARG:HG3	2:B:266:LYS:HG3	1.79	0.65
1:K:91:ILE:O	1:K:91:ILE:HD12	1.96	0.65
1:C:339:GLU:O	1:C:343:ILE:HG13	1.97	0.65
1:A:97:ARG:HG2	1:A:101:ASP:OD2	1.97	0.65
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.27	0.65
2:B:69:LYS:O	2:B:73:ILE:HG13	1.97	0.65
1:K:330:LYS:HE2	1:K:367:HIS:HB3	1.79	0.65
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.79	0.64
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.62	0.64
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.80	0.64
1:A:91:ILE:O	1:A:91:ILE:HD12	1.97	0.64
2:D:212:GLN:NE2	2:D:222:SER:HB3	2.12	0.64
1:A:339:GLU:O	1:A:343:ILE:HG13	1.98	0.64
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.12	0.64
2:D:263:ARG:HG3	2:D:266:LYS:HG3	1.80	0.64
2:F:26:VAL:O	2:F:30:GLN:HG3	1.98	0.64
2:J:87:ARG:HH12	2:J:90:LEU:HD11	1.61	0.64
2:D:318:ASP:HB2	7:N:1208:GER:H71	1.79	0.64
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.63	0.63
1:G:261:GLN:O	1:G:265:GLU:HG2	1.99	0.63
2:H:263:ARG:HG3	2:H:266:LYS:HG3	1.79	0.63
2:F:263:ARG:HG3	2:F:266:LYS:HG3	1.79	0.63
2:H:69:LYS:O	2:H:73:ILE:HG13	1.99	0.63
2:F:69:LYS:O	2:F:73:ILE:HG13	1.99	0.63
2:B:92:ARG:NH1	2:B:119:SER:HB3	2.13	0.63
2:L:263:ARG:HG3	2:L:266:LYS:HG3	1.80	0.62
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.82	0.62
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.81	0.62
1:G:100:TYR:O	1:G:104:ARG:HG3	1.98	0.62
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:209:VAL:N	7:N:1208:GER:H11	2.14	0.62
2:H:318:ASP:HB2	7:P:1408:GER:H71	1.80	0.62
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.00	0.62
1:I:69:ARG:HB3	1:I:71:GLU:OE1	2.00	0.61
1:G:334:LEU:HD22	1:G:367:HIS:O	2.00	0.61
2:H:245:LEU:O	2:H:249:LYS:HG3	2.00	0.61
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.66	0.61
1:A:328:ASP:O	1:A:329:ASN:HB2	2.00	0.61
1:E:91:ILE:O	1:E:91:ILE:HD12	2.00	0.61
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.82	0.60
2:H:349:ARG:O	2:H:352:GLU:HB2	2.01	0.60
1:C:91:ILE:O	1:C:91:ILE:HD12	2.01	0.60
2:D:353:ARG:HH11	2:D:357:LEU:HG	1.64	0.60
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.83	0.60
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.66	0.60
2:L:210:LEU:HB2	2:L:223:THR:HA	1.83	0.60
2:H:21:LEU:HD23	2:H:24:ARG:HE	1.66	0.60
1:A:214:ARG:O	1:A:214:ARG:HG3	2.01	0.60
2:D:39:ARG:H	2:D:39:ARG:CD	2.14	0.60
3:M:109:VAL:N	7:M:1108:GER:H11	2.17	0.60
3:Q:509:VAL:N	7:Q:1508:GER:H11	2.17	0.60
2:H:210:LEU:HB2	2:H:223:THR:HA	1.83	0.59
3:O:309:VAL:N	7:O:1308:GER:H11	2.18	0.59
2:J:210:LEU:HB2	2:J:223:THR:HA	1.82	0.59
1:C:78:VAL:HB	1:C:104:ARG:HB3	1.83	0.59
2:L:318:ASP:HB2	7:R:1608:GER:H71	1.85	0.59
2:B:212:GLN:NE2	2:B:222:SER:HB3	2.18	0.59
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.85	0.59
1:I:207:GLN:HG2	1:I:242:PHE:CE2	2.38	0.58
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.38	0.58
2:B:210:LEU:HB2	2:B:223:THR:HA	1.85	0.58
1:E:318:ILE:HG22	1:E:322:MET:CE	2.33	0.58
2:B:92:ARG:HH11	2:B:119:SER:HB3	1.67	0.58
3:P:409:VAL:N	7:P:1408:GER:H11	2.17	0.58
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.69	0.58
3:R:609:VAL:N	7:R:1608:GER:H11	2.19	0.58
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.85	0.58
1:I:334:LEU:HD22	1:I:367:HIS:O	2.03	0.58
1:K:293:PRO:HD3	8:K:1527:HOH:O	2.03	0.58
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.85	0.58
1:K:311:LEU:HD23	1:K:311:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.85	0.58
2:F:210:LEU:HB2	2:F:223:THR:HA	1.86	0.57
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.18	0.57
1:K:334:LEU:HD22	1:K:367:HIS:O	2.03	0.57
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.38	0.57
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.86	0.57
1:E:265:GLU:O	1:E:269:LEU:HD13	2.05	0.57
2:D:210:LEU:HB2	2:D:223:THR:HA	1.85	0.57
2:H:339:LYS:HG2	2:H:348:THR:CG2	2.34	0.57
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.70	0.57
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.86	0.57
2:B:26:VAL:O	2:B:30:GLN:HG3	2.03	0.57
2:L:353:ARG:HD3	2:L:353:ARG:O	2.05	0.57
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.69	0.57
2:H:339:LYS:HG2	2:H:348:THR:HG21	1.86	0.57
1:E:214:ARG:O	1:E:214:ARG:CG	2.53	0.56
3:P:409:VAL:HG23	3:P:410:ILE:HG23	1.87	0.56
1:E:339:GLU:O	1:E:343:ILE:HG13	2.05	0.56
2:J:27:ARG:HH12	2:J:30:GLN:NE2	2.03	0.56
1:K:192:ILE:O	1:K:195:GLN:HG3	2.05	0.56
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.87	0.56
1:G:330:LYS:HE2	1:G:367:HIS:HB3	1.87	0.56
2:J:87:ARG:NH1	2:J:90:LEU:HD11	2.21	0.55
2:H:92:ARG:HG2	2:H:165:PRO:HG3	1.88	0.55
3:M:109:VAL:HG23	3:M:110:ILE:HG23	1.88	0.55
1:I:328:ASP:O	1:I:329:ASN:HB2	2.05	0.55
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.41	0.55
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.55
1:K:198:LYS:HD3	2:L:266:LYS:HD3	1.89	0.55
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.41	0.55
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.05	0.55
1:E:261:GLN:O	1:E:265:GLU:HG2	2.06	0.55
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.71	0.55
2:B:22:ARG:HH11	2:B:22:ARG:HG2	1.72	0.55
1:C:330:LYS:HE2	1:C:367:HIS:HB3	1.87	0.55
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.71	0.55
1:A:265:GLU:O	1:A:269:LEU:HD13	2.07	0.55
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.03	0.55
3:R:609:VAL:HG23	3:R:610:ILE:HG23	1.89	0.55
1:I:330:LYS:HE2	1:I:367:HIS:HB3	1.89	0.54
3:Q:509:VAL:HG23	3:Q:510:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:265:GLU:O	1:K:269:LEU:HD13	2.06	0.54
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.54
1:I:311:LEU:C	1:I:311:LEU:HD23	2.28	0.54
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.90	0.54
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.90	0.54
1:A:285:GLN:NE2	2:B:247:ARG:NH1	2.56	0.54
2:H:26:VAL:O	2:H:30:GLN:HG3	2.07	0.54
1:E:78:VAL:O	1:E:104:ARG:HD2	2.08	0.54
1:I:100:TYR:O	1:I:104:ARG:HG3	2.08	0.54
2:D:37:PRO:HB3	2:D:39:ARG:HH11	1.72	0.53
2:J:22:ARG:O	2:J:26:VAL:HG23	2.08	0.53
1:E:58:LEU:HD22	1:E:95:LYS:HD3	1.91	0.53
1:G:334:LEU:O	1:G:338:LEU:HG	2.09	0.53
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.90	0.53
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.90	0.53
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.88	0.53
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.90	0.53
2:B:39:ARG:HH11	2:B:39:ARG:CB	2.18	0.53
1:C:334:LEU:HD22	1:C:367:HIS:O	2.08	0.53
1:A:334:LEU:HD22	1:A:367:HIS:O	2.07	0.53
1:K:311:LEU:HD23	1:K:311:LEU:C	2.28	0.53
2:J:212:GLN:HE21	2:J:222:SER:CB	2.12	0.52
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.92	0.52
2:F:332:MET:HB2	8:F:1537:HOH:O	2.08	0.52
1:I:339:GLU:O	1:I:343:ILE:HG13	2.08	0.52
1:E:92:TYR:O	1:E:97:ARG:NH2	2.42	0.52
1:C:328:ASP:O	1:C:329:ASN:HB2	2.09	0.52
1:A:78:VAL:O	1:A:104:ARG:HD2	2.08	0.52
2:D:22:ARG:HG2	2:D:22:ARG:HH11	1.74	0.52
2:F:30:GLN:O	2:F:34:GLN:HG3	2.10	0.52
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.74	0.52
3:O:309:VAL:HG23	3:O:310:ILE:HG23	1.91	0.52
2:B:245:LEU:O	2:B:249:LYS:HG3	2.10	0.52
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.90	0.52
1:I:198:LYS:HD3	2:J:266:LYS:HD3	1.92	0.52
1:G:339:GLU:O	1:G:343:ILE:HG13	2.09	0.52
2:H:202:ARG:HG3	2:H:202:ARG:NH1	2.26	0.51
2:D:26:VAL:O	2:D:30:GLN:HG3	2.10	0.51
1:K:339:GLU:O	1:K:343:ILE:HG13	2.10	0.51
1:G:265:GLU:O	1:G:269:LEU:HD13	2.11	0.51
1:C:265:GLU:O	1:C:269:LEU:HD13	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:ASP:HB2	8:G:1440:HOH:O	2.10	0.51
2:H:318:ASP:HB2	7:P:1408:GER:C7	2.40	0.51
2:J:258:ASN:OD1	2:J:259:GLY:N	2.37	0.51
3:N:209:VAL:HG23	3:N:210:ILE:HG23	1.92	0.51
2:B:229:SER:O	2:B:233:MET:HG3	2.11	0.51
2:D:258:ASN:OD1	2:D:259:GLY:N	2.39	0.51
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.10	0.51
1:I:265:GLU:O	1:I:269:LEU:HD13	2.11	0.51
3:R:608:CYS:HA	7:R:1608:GER:C2	2.41	0.50
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.10	0.50
1:K:79:PRO:HA	1:K:101:ASP:OD1	2.11	0.50
2:D:37:PRO:CB	2:D:39:ARG:HH11	2.24	0.50
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.93	0.50
2:J:63:SER:O	2:J:66:VAL:HG22	2.11	0.50
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.93	0.50
2:B:21:LEU:HD11	2:B:304:ARG:NH2	2.26	0.50
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.94	0.50
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.77	0.50
1:A:214:ARG:CG	1:A:214:ARG:O	2.58	0.50
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.47	0.50
1:G:198:LYS:HD3	2:H:266:LYS:HD3	1.94	0.49
2:J:27:ARG:NH1	2:J:30:GLN:NE2	2.60	0.49
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.27	0.49
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.94	0.49
1:G:311:LEU:HD23	1:G:311:LEU:C	2.33	0.49
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.93	0.49
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.47	0.49
1:K:303:GLN:O	1:K:307:SER:HB2	2.12	0.49
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.76	0.49
2:J:144:LYS:HG2	2:J:185:LEU:HD22	1.94	0.49
1:C:303:GLN:O	1:C:307:SER:HB2	2.11	0.49
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.85	0.49
2:H:348:THR:HA	2:H:351:SER:OG	2.13	0.49
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	0.49
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.43	0.49
1:I:151:GLU:HG3	1:I:175:LEU:HD11	1.94	0.49
1:C:91:ILE:HD11	2:D:38:GLU:H	1.77	0.49
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.48	0.49
1:G:303:GLN:O	1:G:307:SER:HB2	2.13	0.49
1:E:294:ASN:O	1:E:298:GLN:HG3	2.13	0.48
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.48	0.48
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.95	0.48
2:H:19:ASP:H	2:H:304:ARG:HH21	1.61	0.48
2:D:348:THR:HA	2:D:351:SER:OG	2.13	0.48
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.29	0.48
2:H:130:SER:O	2:H:134:ILE:HG13	2.13	0.48
2:B:64:LEU:HD11	2:B:134:ILE:HG22	1.96	0.48
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.95	0.48
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.49	0.48
2:B:22:ARG:NH1	2:B:22:ARG:HG2	2.29	0.48
1:A:151:GLU:HG3	1:A:175:LEU:HD11	1.96	0.48
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.49	0.48
1:E:67:ARG:NH2	1:E:94:GLU:OE1	2.46	0.48
2:B:29:PHE:O	2:B:33:LEU:HD22	2.14	0.48
2:H:338:CYS:HB3	8:H:1551:HOH:O	2.14	0.47
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.96	0.47
1:K:223:VAL:HG11	1:K:240:ARG:HB2	1.96	0.47
1:C:214:ARG:HG2	1:C:214:ARG:O	2.14	0.47
2:D:333:GLU:O	1:K:357:ARG:NH2	2.47	0.47
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.94	0.47
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.95	0.47
2:B:38:GLU:HG2	2:B:38:GLU:O	2.14	0.47
1:G:90:ILE:HD13	2:H:40:TYR:O	2.14	0.47
2:F:130:SER:O	2:F:134:ILE:HG13	2.14	0.47
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.49	0.47
1:C:105:ALA:O	1:C:109:ARG:HG3	2.14	0.47
3:R:608:CYS:HB3	8:R:1002:HOH:O	2.14	0.47
2:F:64:LEU:HD11	2:F:134:ILE:HG22	1.97	0.47
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.96	0.47
2:H:258:ASN:OD1	2:H:259:GLY:N	2.41	0.47
2:D:86:ASP:N	2:D:86:ASP:OD2	2.44	0.47
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.14	0.47
1:I:325:ASN:O	1:I:326:GLN:C	2.52	0.47
1:G:328:ASP:O	1:G:329:ASN:HB2	2.14	0.47
1:E:334:LEU:HD22	1:E:367:HIS:O	2.14	0.47
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.50	0.47
2:L:333:GLU:HA	8:L:1636:HOH:O	2.15	0.47
1:K:353:LYS:HB2	1:K:353:LYS:HE3	1.68	0.47
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.96	0.47
1:A:91:ILE:HD11	2:B:38:GLU:H	1.79	0.47
2:H:29:PHE:O	2:H:33:LEU:HD22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.80	0.47
2:J:318:ASP:HB2	7:Q:1508:GER:C7	2.45	0.47
1:A:325:ASN:O	1:A:326:GLN:C	2.53	0.47
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.96	0.47
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.50	0.47
2:J:133:ILE:HG22	2:J:350:THR:HG23	1.97	0.46
1:G:353:LYS:HG2	1:G:354:GLU:N	2.29	0.46
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.51	0.46
1:K:328:ASP:O	1:K:329:ASN:HB2	2.15	0.46
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.81	0.46
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.30	0.46
1:G:91:ILE:HD12	2:H:38:GLU:HB2	1.98	0.46
1:A:104:ARG:NH2	8:A:389:HOH:O	2.49	0.46
2:H:22:ARG:NH1	2:H:22:ARG:HG2	2.30	0.46
1:G:173:ARG:HD2	8:G:1452:HOH:O	2.14	0.46
1:G:325:ASN:O	1:G:326:GLN:C	2.54	0.46
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.50	0.46
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.50	0.46
2:D:22:ARG:HG2	2:D:22:ARG:NH1	2.30	0.46
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.51	0.46
2:J:130:SER:O	2:J:134:ILE:HG13	2.16	0.46
2:B:207:ASP:O	2:B:208:ASN:HB2	2.16	0.46
2:H:21:LEU:CD1	2:H:21:LEU:N	2.78	0.46
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.98	0.46
2:F:38:GLU:O	2:F:38:GLU:HG2	2.16	0.46
3:R:608:CYS:C	7:R:1608:GER:H11	2.36	0.46
2:B:130:SER:O	2:B:134:ILE:HG13	2.15	0.46
2:F:333:GLU:HA	8:F:1569:HOH:O	2.14	0.46
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.81	0.46
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.98	0.46
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.51	0.46
2:D:250:ARG:O	2:D:254:MET:HG2	2.16	0.46
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.97	0.46
1:C:104:ARG:HG2	2:D:101:LEU:O	2.15	0.46
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.97	0.46
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.51	0.46
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.51	0.46
2:F:62:ASP:HA	2:F:349:ARG:HH22	1.81	0.46
1:E:353:LYS:CE	1:E:357:ARG:HH22	2.28	0.45
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.97	0.45
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:ARG:HG2	1:E:287:ARG:H	1.49	0.45
2:H:18:LEU:HA	2:H:304:ARG:HH22	1.74	0.45
1:E:296:LEU:HD22	1:E:322:MET:CE	2.46	0.45
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.98	0.45
2:B:24:ARG:HD3	2:B:27:ARG:NH2	2.28	0.45
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.99	0.45
2:B:92:ARG:NH1	2:B:118:ASP:O	2.50	0.45
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.52	0.45
1:C:311:LEU:HD23	1:C:311:LEU:C	2.37	0.45
2:H:202:ARG:HD2	8:H:1547:HOH:O	2.16	0.45
3:R:608:CYS:CB	8:R:1002:HOH:O	2.64	0.45
2:J:27:ARG:HD3	8:J:1564:HOH:O	2.16	0.45
2:J:27:ARG:HH12	2:J:30:GLN:HE22	1.63	0.45
1:G:350:THR:O	1:G:353:LYS:HB3	2.15	0.45
1:A:311:LEU:HD23	1:A:311:LEU:C	2.36	0.45
1:E:274:GLU:HG3	1:E:310:TYR:CE2	2.52	0.45
1:A:287:ARG:O	1:A:291:ARG:HD3	2.17	0.45
1:A:303:GLN:O	1:A:307:SER:HB2	2.16	0.45
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.17	0.45
2:H:207:ASP:O	2:H:208:ASN:HB2	2.17	0.45
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.51	0.45
2:B:250:ARG:O	2:B:254:MET:HG2	2.15	0.45
2:D:130:SER:O	2:D:134:ILE:HG13	2.16	0.45
1:G:290:SER:HB2	1:G:322:MET:HG2	1.99	0.45
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.52	0.45
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.52	0.45
2:H:18:LEU:N	2:H:18:LEU:CD2	2.79	0.45
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.52	0.45
2:D:64:LEU:HD11	2:D:134:ILE:HG22	1.98	0.45
1:K:151:GLU:HG3	1:K:175:LEU:HD11	1.98	0.45
3:O:308:CYS:C	7:O:1308:GER:H11	2.37	0.45
1:G:91:ILE:HD11	2:H:38:GLU:H	1.82	0.45
3:P:408:CYS:C	7:P:1408:GER:H11	2.38	0.44
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.52	0.44
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.52	0.44
2:D:295:ARG:NH1	2:D:299:LEU:CD1	2.80	0.44
1:A:340:LEU:HD23	1:A:343:ILE:HD12	2.00	0.44
2:D:333:GLU:HA	8:D:1561:HOH:O	2.17	0.44
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.52	0.44
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.99	0.44
1:A:357:ARG:HH11	1:A:357:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:TYR:O	1:E:104:ARG:HG3	2.18	0.44
2:H:74:GLU:CD	2:H:141:ARG:HH22	2.21	0.44
2:F:245:LEU:O	2:F:249:LYS:HG3	2.17	0.44
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.52	0.44
1:I:303:GLN:O	1:I:307:SER:HB2	2.17	0.44
2:J:207:ASP:O	2:J:208:ASN:HB2	2.17	0.44
2:F:192:ASP:OD1	2:F:195:LYS:HG3	2.17	0.44
1:I:287:ARG:H	1:I:287:ARG:HG2	1.56	0.44
1:K:97:ARG:HG2	1:K:101:ASP:OD2	2.18	0.44
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.98	0.44
2:B:160:SER:HB3	2:B:199:TYR:CE1	2.53	0.44
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.77	0.44
1:G:215:LEU:HA	8:G:1449:HOH:O	2.17	0.44
2:D:38:GLU:HG2	2:D:38:GLU:O	2.17	0.44
2:B:21:LEU:CD1	2:B:21:LEU:N	2.81	0.44
1:I:58:LEU:HD12	1:I:125:GLU:OE2	2.18	0.44
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.52	0.44
1:C:344:LEU:HD13	1:C:356:TRP:CE2	2.53	0.44
1:E:223:VAL:HG11	1:E:240:ARG:HB2	2.00	0.44
2:F:27:ARG:HA	2:F:30:GLN:HE21	1.83	0.44
2:H:40:TYR:CE2	7:P:1408:GER:H101	2.52	0.44
2:F:353:ARG:NE	8:F:1557:HOH:O	2.49	0.44
2:J:69:LYS:O	2:J:73:ILE:HG13	2.17	0.43
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.53	0.43
2:F:250:ARG:O	2:F:254:MET:HG2	2.17	0.43
2:D:104:PRO:HG2	8:D:1593:HOH:O	2.17	0.43
2:B:295:ARG:HD3	8:B:1549:HOH:O	2.18	0.43
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.54	0.43
1:K:156:ILE:HD12	8:K:1585:HOH:O	2.18	0.43
1:A:92:TYR:O	1:A:97:ARG:NH2	2.50	0.43
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.18	0.43
1:E:121:ARG:NH1	1:E:121:ARG:HG3	2.33	0.43
2:L:250:ARG:O	2:L:254:MET:HG2	2.19	0.43
1:E:303:GLN:O	1:E:307:SER:HB2	2.17	0.43
1:G:65:LEU:O	1:G:69:ARG:HG3	2.19	0.43
1:K:348:LYS:HD2	8:K:1541:HOH:O	2.18	0.43
2:F:70:ASP:O	2:F:74:GLU:HG2	2.19	0.43
2:H:352:GLU:HA	2:H:352:GLU:OE2	2.19	0.43
1:A:303:GLN:N	1:A:304:PRO:CD	2.82	0.43
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.53	0.43
2:D:115:HIS:ND1	2:D:116:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:ASN:OD1	2:B:259:GLY:N	2.47	0.43
2:B:258:ASN:CG	2:B:259:GLY:H	2.22	0.43
2:D:256:GLN:HB2	2:D:260:TYR:CE2	2.53	0.43
2:B:103:ILE:HG23	2:B:104:PRO:HD2	2.00	0.43
2:H:133:ILE:HG22	2:H:350:THR:HG23	2.00	0.43
2:L:110:ASN:CB	2:L:111:PRO:HD2	2.49	0.43
1:K:287:ARG:HG2	1:K:287:ARG:H	1.56	0.43
6:L:1506:GRG:H101	6:L:1506:GRG:HC62	1.88	0.43
1:C:287:ARG:H	1:C:287:ARG:HG2	1.63	0.43
3:N:208:CYS:C	7:N:1208:GER:H11	2.38	0.42
1:I:223:VAL:HG11	1:I:240:ARG:HB2	2.01	0.42
2:H:341:HIS:HA	2:H:342:PRO:HD2	1.84	0.42
2:F:207:ASP:O	2:F:208:ASN:HB2	2.18	0.42
2:J:19:ASP:OD2	2:J:19:ASP:N	2.52	0.42
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.34	0.42
2:B:318:ASP:HB2	7:M:1108:GER:C7	2.47	0.42
2:F:318:ASP:HB2	7:O:1308:GER:C7	2.47	0.42
1:K:329:ASN:HB3	1:K:332:ASP:HB3	2.01	0.42
1:C:325:ASN:O	1:C:326:GLN:C	2.57	0.42
1:E:325:ASN:O	1:E:326:GLN:C	2.56	0.42
2:B:269:ASP:C	2:B:269:ASP:OD1	2.58	0.42
8:H:1560:HOH:O	3:P:409:VAL:HG21	2.19	0.42
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.54	0.42
2:B:19:ASP:N	2:B:19:ASP:OD2	2.51	0.42
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.54	0.42
1:E:312:ILE:O	1:E:316:VAL:HG23	2.20	0.42
2:J:121:HIS:HB3	2:J:124:MET:HG2	2.02	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.91	0.42
2:D:19:ASP:OD2	2:D:19:ASP:N	2.43	0.42
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.84	0.42
7:O:1308:GER:H91	7:O:1308:GER:H112	1.87	0.42
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.46	0.42
1:E:303:GLN:N	1:E:304:PRO:CD	2.82	0.42
1:K:325:ASN:O	1:K:326:GLN:C	2.57	0.42
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.02	0.42
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.49	0.42
2:H:250:ARG:O	2:H:254:MET:HG2	2.20	0.42
2:J:237:GLU:HG2	8:J:1534:HOH:O	2.20	0.42
2:B:115:HIS:HA	2:B:116:PRO:HD3	1.86	0.42
2:J:30:GLN:HE21	2:J:30:GLN:HB3	1.63	0.42
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1502:GRG:H101	6:D:1502:GRG:HC62	1.92	0.42
2:D:19:ASP:O	2:D:21:LEU:HD13	2.20	0.42
2:D:121:HIS:HB3	2:D:124:MET:HG2	2.02	0.42
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.55	0.42
2:H:269:ASP:C	2:H:269:ASP:OD1	2.59	0.42
3:Q:508:CYS:C	7:Q:1508:GER:H11	2.39	0.42
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.55	0.42
1:E:338:LEU:HD11	1:E:364:GLN:HG3	2.01	0.42
1:A:71:GLU:CD	1:A:71:GLU:H	2.14	0.42
3:M:108:CYS:C	7:M:1108:GER:H11	2.39	0.41
1:G:318:ILE:HG22	1:G:322:MET:HE3	2.01	0.41
2:J:229:SER:O	2:J:233:MET:HG3	2.20	0.41
2:D:236:LEU:HD22	2:D:245:LEU:HD21	2.02	0.41
6:F:1503:GRG:H101	6:F:1503:GRG:HC62	1.90	0.41
3:P:408:CYS:HA	7:P:1408:GER:C2	2.50	0.41
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.51	0.41
1:A:285:GLN:HE21	2:B:247:ARG:NH1	2.18	0.41
2:B:334:GLU:HB3	2:B:337:ILE:HD12	2.02	0.41
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.54	0.41
1:G:135:HIS:CD2	2:H:166:GLU:HG2	2.55	0.41
1:A:198:LYS:CD	2:B:266:LYS:HD3	2.51	0.41
1:A:251:SER:HA	1:A:287:ARG:HH22	1.85	0.41
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.55	0.41
2:F:29:PHE:O	2:F:33:LEU:HD22	2.20	0.41
2:J:33:LEU:HD22	2:J:54:ALA:HB1	2.02	0.41
3:O:308:CYS:HA	7:O:1308:GER:C2	2.50	0.41
1:G:78:VAL:O	1:G:104:ARG:HD2	2.21	0.41
2:H:353:ARG:O	2:H:357:LEU:HB2	2.20	0.41
1:G:318:ILE:HG22	1:G:322:MET:CE	2.51	0.41
1:I:96:PHE:CE1	1:I:126:LEU:HB3	2.55	0.41
2:L:243:LYS:HB2	2:L:243:LYS:HE3	1.91	0.41
1:G:149:GLN:HG3	8:G:1443:HOH:O	2.19	0.41
2:J:64:LEU:O	2:J:67:VAL:HG22	2.19	0.41
1:C:244:ILE:HD11	1:C:259:GLU:OE1	2.21	0.41
7:N:1208:GER:H91	7:N:1208:GER:H112	1.89	0.41
2:H:357:LEU:HD22	2:H:361:TRP:CE2	2.56	0.41
2:L:69:LYS:O	2:L:73:ILE:HG13	2.21	0.41
2:B:110:ASN:CB	2:B:111:PRO:HD2	2.50	0.41
1:I:67:ARG:HD2	8:I:462:HOH:O	2.20	0.41
2:D:53:PHE:HE1	7:N:1208:GER:H42	1.86	0.41
7:R:1608:GER:H91	7:R:1608:GER:H112	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ILE:HD13	1:C:134:TRP:CH2	2.56	0.41
2:J:245:LEU:O	2:J:249:LYS:HG3	2.21	0.41
1:A:294:ASN:O	1:A:298:GLN:HG3	2.20	0.41
2:J:36:LEU:HA	2:J:37:PRO:HD3	1.91	0.41
1:E:328:ASP:O	1:E:329:ASN:HB2	2.21	0.41
2:H:86:ASP:N	2:H:86:ASP:OD2	2.54	0.41
3:M:108:CYS:HA	7:M:1108:GER:C2	2.51	0.40
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.50	0.40
2:F:18:LEU:HD12	2:F:304:ARG:NH1	2.36	0.40
1:A:71:GLU:O	1:A:115:ARG:NH1	2.54	0.40
1:I:82:ASP:HB2	1:I:86:PRO:HB3	2.02	0.40
1:I:124:ILE:HD13	1:I:134:TRP:CH2	2.56	0.40
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.20	0.40
1:C:78:VAL:O	1:C:104:ARG:HD2	2.21	0.40
1:A:334:LEU:O	1:A:338:LEU:HG	2.22	0.40
1:G:227:LEU:HA	1:G:227:LEU:HD23	1.94	0.40
2:D:101:LEU:HD23	2:D:101:LEU:HA	1.94	0.40
1:E:353:LYS:HE3	1:E:357:ARG:NH2	2.29	0.40
3:R:608:CYS:HA	7:R:1608:GER:H21	2.02	0.40
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.53	0.40
1:C:251:SER:HA	1:C:287:ARG:HH12	1.87	0.40
2:F:53:PHE:HE1	7:O:1308:GER:H42	1.86	0.40
2:D:318:ASP:HB2	7:N:1208:GER:C7	2.47	0.40
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.02	0.40
2:H:33:LEU:HD22	2:H:54:ALA:HB1	2.03	0.40
2:J:86:ASP:OD2	2:J:86:ASP:N	2.54	0.40
1:E:311:LEU:HD23	1:E:311:LEU:C	2.42	0.40
1:G:97:ARG:NH1	1:G:97:ARG:CB	2.85	0.40
2:L:33:LEU:HD22	2:L:54:ALA:HB1	2.04	0.40
1:C:184:GLN:HB2	8:C:1404:HOH:O	2.21	0.40
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:433:HOH:O	8:I:433:HOH:O[2_657]	0.35	1.85

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%)	290 (93%)	20 (6%)	2 (1%)	30	56
1	C	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	46	72
1	E	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	46	72
1	G	312/377 (83%)	294 (94%)	16 (5%)	2 (1%)	30	56
1	I	312/377 (83%)	293 (94%)	17 (5%)	2 (1%)	30	56
1	K	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	46	72
2	B	344/377 (91%)	334 (97%)	9 (3%)	1 (0%)	46	72
2	D	344/377 (91%)	333 (97%)	9 (3%)	2 (1%)	30	56
2	F	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	46	72
2	H	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	21	42
2	J	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	46	72
2	L	344/377 (91%)	333 (97%)	10 (3%)	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
3	O	2/11 (18%)	2 (100%)	0	0	100	100
3	P	2/11 (18%)	2 (100%)	0	0	100	100
3	Q	2/11 (18%)	2 (100%)	0	0	100	100
3	R	3/11 (27%)	3 (100%)	0	0	100	100
All	All	3949/4590 (86%)	3756 (95%)	175 (4%)	18 (0%)	34	60

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	G	326	GLN
2	B	258	ASN
1	C	326	GLN

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Mol	Chain	Res	Type
2	D	258	ASN
2	F	258	ASN
2	H	258	ASN
1	I	326	GLN
2	J	258	ASN
2	L	258	ASN
1	E	326	GLN
1	G	306	HIS
2	H	333	GLU
1	I	306	HIS
1	K	306	HIS
2	D	333	GLU
1	A	306	HIS
2	H	111	PRO

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	90
1	C	283/338 (84%)	273 (96%)	10 (4%)	43	71
1	E	284/338 (84%)	275 (97%)	9 (3%)	46	74
1	G	281/338 (83%)	277 (99%)	4 (1%)	74	90
1	I	287/338 (85%)	280 (98%)	7 (2%)	57	82
1	K	291/338 (86%)	283 (97%)	8 (3%)	52	79
2	B	289/326 (89%)	276 (96%)	13 (4%)	34	62
2	D	293/326 (90%)	277 (94%)	16 (6%)	27	51
2	F	294/326 (90%)	280 (95%)	14 (5%)	31	58
2	H	288/326 (88%)	274 (95%)	14 (5%)	31	57
2	J	292/326 (90%)	277 (95%)	15 (5%)	29	55
2	L	296/326 (91%)	280 (95%)	16 (5%)	27	52
3	M	4/11 (36%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	N	4/11 (36%)	4 (100%)	0	100 100
3	O	4/11 (36%)	4 (100%)	0	100 100
3	P	4/11 (36%)	4 (100%)	0	100 100
3	Q	4/11 (36%)	4 (100%)	0	100 100
3	R	5/11 (46%)	5 (100%)	0	100 100
All	All	3483/4050 (86%)	3353 (96%)	130 (4%)	41 69

All (130) 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	33	LEU
2	B	39	ARG
2	B	113	THR
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU
2	B	255	ARG
2	B	258	ASN
2	B	261	HIS
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	76	ASP
1	C	81	ASN
1	C	182	PRO
1	C	217	ASP
1	C	287	ARG
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	27	ARG
2	D	33	LEU

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Mol	Chain	Res	Type
2	D	39	ARG
2	D	110	ASN
2	D	151	LEU
2	D	216	LEU
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
1	E	67	ARG
1	E	71	GLU
1	E	81	ASN
1	E	191	ASP
1	E	214	ARG
1	E	257	GLU
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	24	ARG
2	F	33	LEU
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	353	LYS
2	H	18	LEU
2	H	21	LEU

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Mol	Chain	Res	Type
2	H	91	ASP
2	H	151	LEU
2	H	216	LEU
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	357	LEU
1	I	55	PHE
1	I	67	ARG
1	I	71	GLU
1	I	142	ARG
1	I	194	ASN
1	I	287	ARG
1	I	364	GLN
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	33	LEU
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
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	59	ASP
1	K	71	GLU
1	K	142	ARG
1	K	194	ASN
1	K	195	GLN
1	K	287	ARG
1	K	324	GLU

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Mol	Chain	Res	Type
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	284	LYS
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 (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	184	GLN
1	A	201	HIS
1	A	285	GLN
1	A	329	ASN
1	A	335	ASN
2	B	208	ASN
1	C	108	GLN
1	C	201	HIS
1	C	218	ASN
1	C	298	GLN
1	C	364	GLN
2	D	246	ASN
1	E	184	GLN
1	E	201	HIS
1	E	298	GLN
1	E	335	ASN
2	F	30	GLN
2	F	212	GLN
2	F	246	ASN
1	G	80	GLN
1	G	89	GLN

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Mol	Chain	Res	Type
1	G	153	ASN
1	G	162	GLN
1	G	201	HIS
1	G	297	ASN
1	G	325	ASN
1	I	89	GLN
1	I	195	GLN
1	I	201	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	81	ASN
1	K	201	HIS
1	K	298	GLN
1	K	325	ASN
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 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 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	1501	-	26,28,28	0.84	1 (3%)	33,37,37	0.86	0
6	GRG	D	1502	-	26,28,28	0.87	2 (7%)	33,37,37	0.85	0
6	GRG	F	1503	-	26,28,28	0.84	0	33,37,37	0.87	0
6	GRG	H	1504	-	26,28,28	0.84	0	33,37,37	0.85	0
6	GRG	J	1505	-	26,28,28	0.83	0	33,37,37	0.84	0
6	GRG	L	1506	-	26,28,28	0.78	0	33,37,37	0.87	0
7	GER	M	1108	3	19,19,19	1.05	1 (5%)	22,22,22	0.73	0
7	GER	N	1208	3	19,19,19	1.05	2 (10%)	22,22,22	0.73	0
7	GER	O	1308	3	19,19,19	1.06	1 (5%)	22,22,22	0.73	0
7	GER	P	1408	3	19,19,19	1.04	1 (5%)	22,22,22	0.70	0
7	GER	Q	1508	3	19,19,19	1.02	2 (10%)	22,22,22	0.73	0
7	GER	R	1608	3	19,19,19	1.03	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	1501	-	-	0/31/31/31	0/0/0/0
6	GRG	D	1502	-	-	0/31/31/31	0/0/0/0
6	GRG	F	1503	-	-	0/31/31/31	0/0/0/0
6	GRG	H	1504	-	-	0/31/31/31	0/0/0/0
6	GRG	J	1505	-	-	0/31/31/31	0/0/0/0
6	GRG	L	1506	-	-	0/31/31/31	0/0/0/0
7	GER	M	1108	3	-	0/20/20/20	0/0/0/0
7	GER	N	1208	3	-	0/20/20/20	0/0/0/0
7	GER	O	1308	3	-	0/20/20/20	0/0/0/0
7	GER	P	1408	3	-	0/20/20/20	0/0/0/0
7	GER	Q	1508	3	-	0/20/20/20	0/0/0/0
7	GER	R	1608	3	-	0/20/20/20	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	1508	GER	C7-C8	2.01	1.36	1.33
6	B	1501	GRG	C7-C8	2.03	1.36	1.33
6	D	1502	GRG	C7-C8	2.03	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1208	GER	C2-C3	2.07	1.37	1.32
6	D	1502	GRG	C2-C3	2.08	1.37	1.33
7	R	1608	GER	C7-C8	2.09	1.37	1.33
7	R	1608	GER	C12-C13	2.24	1.37	1.33
7	M	1108	GER	C12-C13	2.28	1.37	1.33
7	Q	1508	GER	C12-C13	2.32	1.37	1.33
7	N	1208	GER	C12-C13	2.37	1.37	1.33
7	P	1408	GER	C12-C13	2.38	1.37	1.33
7	O	1308	GER	C12-C13	2.45	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.

12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1501	GRG	1	0
6	D	1502	GRG	2	0
6	F	1503	GRG	2	0
6	H	1504	GRG	1	0
6	J	1505	GRG	1	0
6	L	1506	GRG	2	0
7	M	1108	GER	5	0
7	N	1208	GER	6	0
7	O	1308	GER	7	0
7	P	1408	GER	6	0
7	Q	1508	GER	4	0
7	R	1608	GER	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	-0.06	9 (2%)	55	48	35, 57, 91, 109	0
1	C	314/377 (83%)	-0.11	7 (2%)	65	59	33, 54, 82, 99	0
1	E	314/377 (83%)	0.00	10 (3%)	51	44	33, 58, 86, 104	0
1	G	314/377 (83%)	0.03	8 (2%)	61	54	36, 58, 88, 102	0
1	I	314/377 (83%)	-0.14	6 (1%)	70	64	29, 53, 84, 95	0
1	K	314/377 (83%)	-0.35	3 (0%)	84	81	23, 43, 67, 82	0
2	B	346/377 (91%)	-0.10	7 (2%)	68	63	36, 51, 77, 102	0
2	D	346/377 (91%)	0.02	8 (2%)	64	57	31, 47, 74, 94	0
2	F	346/377 (91%)	-0.12	11 (3%)	51	44	32, 47, 75, 100	0
2	H	346/377 (91%)	0.37	24 (6%)	20	14	37, 65, 95, 113	0
2	J	346/377 (91%)	0.05	14 (4%)	42	34	30, 50, 78, 104	0
2	L	346/377 (91%)	-0.09	8 (2%)	64	57	26, 41, 64, 95	0
3	M	4/11 (36%)	6.75	4 (100%)	0	0	58, 64, 70, 80	4 (100%)
3	N	4/11 (36%)	6.24	4 (100%)	0	0	60, 64, 71, 78	4 (100%)
3	O	4/11 (36%)	7.97	4 (100%)	0	0	58, 64, 70, 80	4 (100%)
3	P	4/11 (36%)	6.21	4 (100%)	0	0	60, 64, 70, 78	4 (100%)
3	Q	4/11 (36%)	5.29	4 (100%)	0	0	58, 63, 72, 81	4 (100%)
3	R	5/11 (45%)	3.46	5 (100%)	0	0	57, 62, 83, 84	5 (100%)
All	All	3985/4590 (86%)	-0.00	140 (3%)	48	40	23, 52, 84, 113	25 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	308	CYS	11.5
3	M	108	CYS	10.3
3	N	208	CYS	8.2

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Mol	Chain	Res	Type	RSRZ
3	M	109	VAL	7.8
3	O	309	VAL	7.3
3	O	310	ILE	7.2
3	P	408	CYS	7.1
3	P	410	ILE	6.6
3	N	211	LEU	6.3
1	C	306	HIS	6.3
2	H	304	ARG	6.1
3	N	210	ILE	6.1
3	Q	510	ILE	6.1
3	Q	508	CYS	6.0
3	O	311	LEU	5.8
3	P	409	VAL	5.8
1	G	306	HIS	5.6
3	M	110	ILE	5.5
3	P	411	LEU	5.4
1	G	55	PHE	5.1
2	L	113	THR	4.9
3	Q	511	LEU	4.8
2	J	108	SER	4.7
1	E	306	HIS	4.6
1	G	305	SER	4.6
2	H	305	LEU	4.5
3	N	209	VAL	4.4
1	C	305	SER	4.3
3	Q	509	VAL	4.3
3	R	610	ILE	4.2
3	R	611	LEU	3.9
2	D	111	PRO	3.8
2	F	113	THR	3.8
2	F	112	GLY	3.7
3	R	609	VAL	3.7
2	H	111	PRO	3.6
2	D	305	LEU	3.6
1	A	306	HIS	3.6
1	C	304	PRO	3.5
1	A	328	ASP	3.5
2	H	108	SER	3.5
2	J	111	PRO	3.4
3	M	111	LEU	3.4
2	H	110	ASN	3.4
2	B	363	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	306	VAL	3.3
2	D	110	ASN	3.3
2	F	314	ASP	3.2
2	D	113	THR	3.2
2	J	85	GLU	3.2
2	L	110	ASN	3.2
2	H	363	THR	3.2
2	L	111	PRO	3.1
2	H	86	ASP	3.1
2	B	86	ASP	3.1
2	J	84	THR	3.1
2	H	88	SER	3.1
2	H	84	THR	3.1
1	I	306	HIS	3.0
2	J	114	ALA	3.0
2	J	86	ASP	3.0
2	B	305	LEU	2.9
1	A	304	PRO	2.9
2	B	113	THR	2.9
3	R	607	LYS	2.9
2	H	87	ARG	2.9
2	B	111	PRO	2.9
2	H	361	TRP	2.8
1	I	328	ASP	2.8
2	L	49	THR	2.8
1	A	330	LYS	2.7
2	F	88	SER	2.7
2	H	307	GLY	2.8
2	H	65	ASP	2.7
1	E	331	GLU	2.7
1	G	304	PRO	2.7
1	I	304	PRO	2.7
2	F	86	ASP	2.7
3	R	608	CYS	2.7
1	C	55	PHE	2.7
2	H	314	ASP	2.7
2	H	316	HIS	2.6
2	H	85	GLU	2.6
2	J	46	SER	2.6
2	L	363	THR	2.6
2	J	112	GLY	2.6
1	C	329	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	314	ASP	2.5
2	H	112	GLY	2.5
2	D	108	SER	2.5
2	L	314	ASP	2.5
2	J	363	THR	2.5
2	D	363	THR	2.5
1	E	304	PRO	2.4
1	E	55	PHE	2.4
2	J	360	SER	2.4
2	H	303	ASP	2.4
1	A	326	GLN	2.4
2	F	111	PRO	2.4
2	H	23	ASP	2.4
1	A	368	SER	2.3
2	F	363	THR	2.3
2	F	305	LEU	2.3
1	E	368	SER	2.3
1	A	342	GLU	2.3
1	C	331	GLU	2.3
2	J	314	ASP	2.3
1	K	306	HIS	2.3
2	D	304	ARG	2.3
1	A	217	ASP	2.3
1	I	368	SER	2.3
2	H	113	THR	2.3
1	I	305	SER	2.2
1	E	328	ASP	2.2
2	B	110	ASN	2.2
1	G	78	VAL	2.2
1	K	304	PRO	2.2
2	B	362	LYS	2.2
2	L	112	GLY	2.1
2	H	40	TYR	2.1
1	K	305	SER	2.1
2	F	110	ASN	2.1
1	E	330	LYS	2.1
1	G	326	GLN	2.1
2	H	83	PRO	2.1
1	C	332	ASP	2.1
1	G	59	ASP	2.1
1	E	326	GLN	2.1
1	G	303	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	367	HIS	2.1
2	F	316	HIS	2.1
2	H	19	ASP	2.1
1	E	367	HIS	2.1
1	E	305	SER	2.1
1	A	333	ILE	2.0
2	J	88	SER	2.0
2	F	46	SER	2.0
2	J	110	ASN	2.0
2	J	49	THR	2.0
2	L	86	ASP	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	1402	1/1	0.97	0.25	8.23	59,59,59,59	0
5	CL	G	1405	1/1	0.96	0.21	5.40	53,53,53,53	0
7	GER	R	1608	20/20	0.72	0.51	2.23	64,72,82,83	20
7	GER	M	1108	20/20	0.50	0.58	1.61	69,76,83,84	20
7	GER	P	1408	20/20	0.52	0.57	1.60	72,78,81,82	20
5	CL	K	1408	1/1	0.98	0.16	1.56	57,57,57,57	0
7	GER	Q	1508	20/20	0.71	0.47	1.47	69,76,84,84	20
7	GER	N	1208	20/20	0.61	0.51	1.42	67,76,84,84	20
7	GER	O	1308	20/20	0.54	0.56	1.26	71,78,83,83	20
6	GRG	B	1501	29/29	0.95	0.27	0.62	56,60,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	GRG	L	1506	29/29	0.95	0.26	0.54	40,45,53,58	0
6	GRG	F	1503	29/29	0.95	0.27	0.36	50,58,70,71	0
6	GRG	D	1502	29/29	0.94	0.27	0.31	49,56,65,66	0
6	GRG	H	1504	29/29	0.94	0.27	0.19	61,65,75,77	0
6	GRG	J	1505	29/29	0.95	0.25	0.16	43,48,56,58	0
5	CL	F	1404	1/1	0.99	0.13	-0.09	47,47,47,47	0
5	CL	B	1401	1/1	0.98	0.13	-0.90	61,61,61,61	0
4	ZN	J	378	1/1	0.99	0.14	-0.93	42,42,42,42	0
4	ZN	D	378	1/1	1.00	0.14	-1.18	45,45,45,45	0
5	CL	J	1407	1/1	0.94	0.13	-1.36	61,61,61,61	0
5	CL	H	1406	1/1	0.96	0.13	-1.53	60,60,60,60	0
5	CL	D	1403	1/1	0.99	0.13	-1.73	43,43,43,43	0
4	ZN	L	378	1/1	1.00	0.12	-1.78	34,34,34,34	0
4	ZN	B	378	1/1	1.00	0.11	-2.18	47,47,47,47	0
4	ZN	F	378	1/1	1.00	0.10	-2.33	47,47,47,47	0
5	CL	L	1409	1/1	0.99	0.07	-2.59	45,45,45,45	0
4	ZN	H	378	1/1	0.99	0.11	-3.22	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.