Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:04 PM GMT

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

This is a 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:

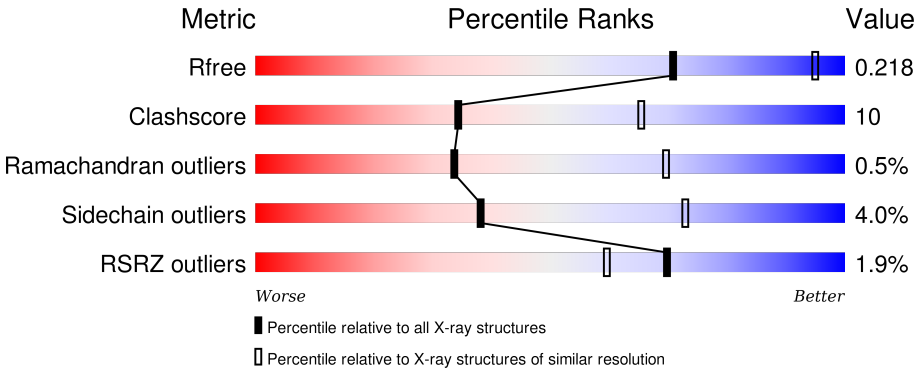
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	64% 19% • 17%
1	C	377	65% 17% • 17%
1	E	377	62% 20% • 17%
1	G	377	65% 17% • 17%
1	I	377	62% 20% • 17%

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Mol	Chain	Length	Quality of chain
1	K	377	65% 17% 17%
2	B	377	2% 71% 19% 8%
2	D	377	2% 67% 21% 8%
2	F	377	2% 71% 20% 8%
2	H	377	3% 69% 21% 8%
2	J	377	2% 71% 19% 8%
2	L	377	% 75% 15% 8%
3	M	11	9% 36% 18% 45%
3	N	11	9% 27% 27% 45%
3	O	11	9% 36% 18% 45%
3	P	11	9% 55% 45%
3	Q	11	36% 18% 45%
3	R	11	36% 18% 45%

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
4	MES	A	901	-	-	-	X
4	MES	C	902	-	-	-	X
4	MES	E	903	-	-	-	X
4	MES	G	904	-	-	-	X
4	MES	I	905	-	-	-	X
4	MES	K	906	-	-	-	X
7	CL	G	804	-	-	X	-
8	GER	M	1108	-	-	-	X
8	GER	R	1608	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33129 atoms, of which 0 are 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
			2614	1673	458	478	5			
1	C	314	Total	C	N	O	S	0	0	0
			2648	1691	462	490	5			
1	E	314	Total	C	N	O	S	0	0	0
			2630	1682	460	483	5			
1	G	314	Total	C	N	O	S	0	0	0
			2632	1683	459	485	5			
1	I	314	Total	C	N	O	S	0	0	0
			2654	1693	461	495	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

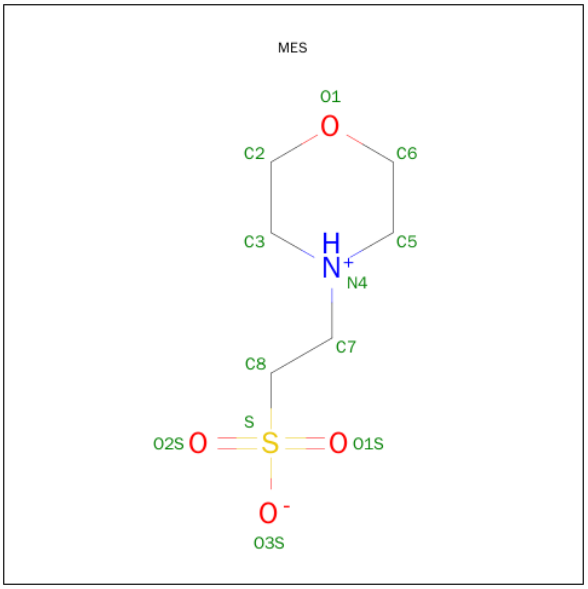
- Molecule 2 is a protein called geranyltransferase type-I beta subunit.

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

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

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

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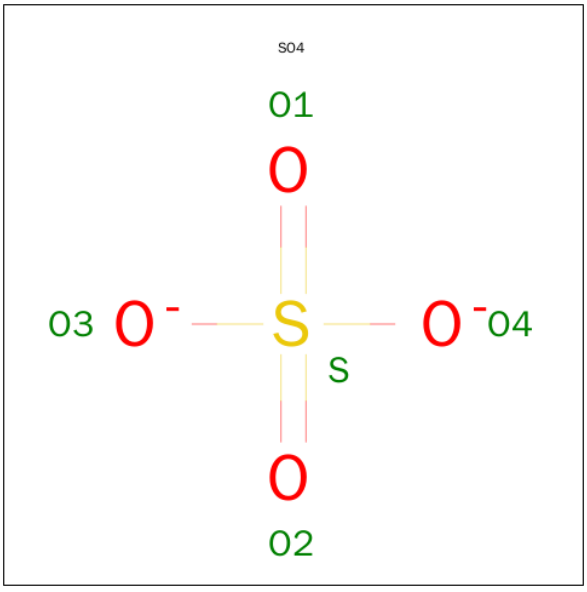
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total C N O S 12 6 1 4 1	0	0

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

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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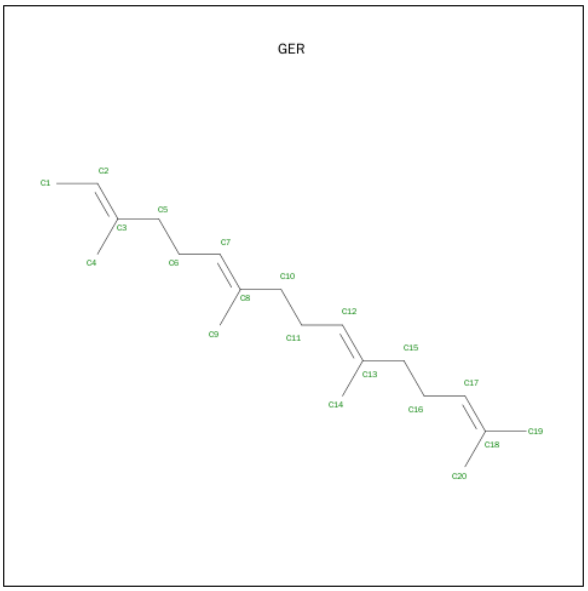
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	J	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0

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

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

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



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

- Molecule 9 is water.

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

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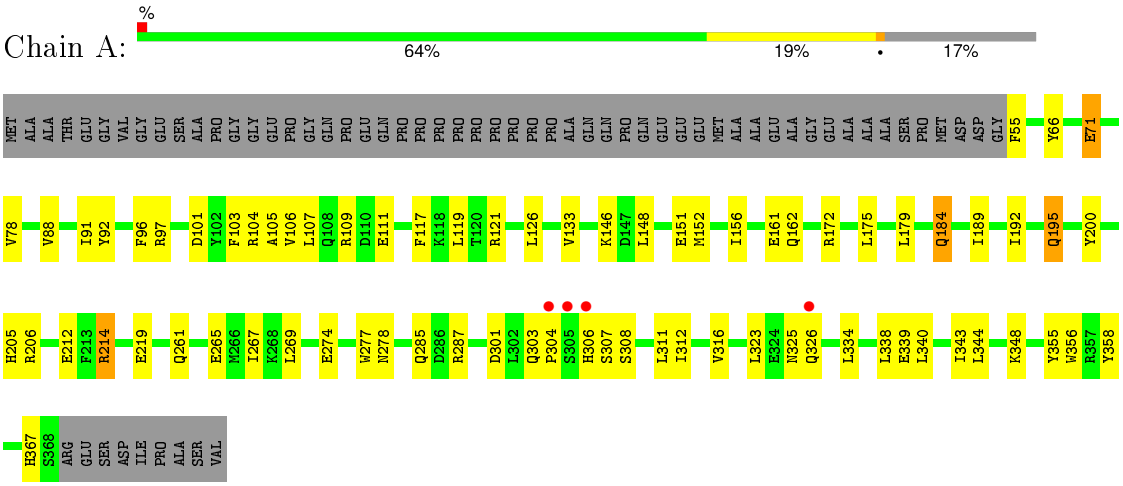
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	40	Total O 40 40	0	0
9	H	23	Total O 23 23	0	0
9	I	52	Total O 52 52	0	0
9	J	36	Total O 36 36	0	0
9	K	101	Total O 101 101	0	0
9	L	60	Total O 60 60	0	0
9	M	1	Total O 1 1	0	0
9	N	3	Total O 3 3	0	0
9	O	1	Total O 1 1	0	0
9	Q	3	Total O 3 3	0	0
9	R	5	Total O 5 5	0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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

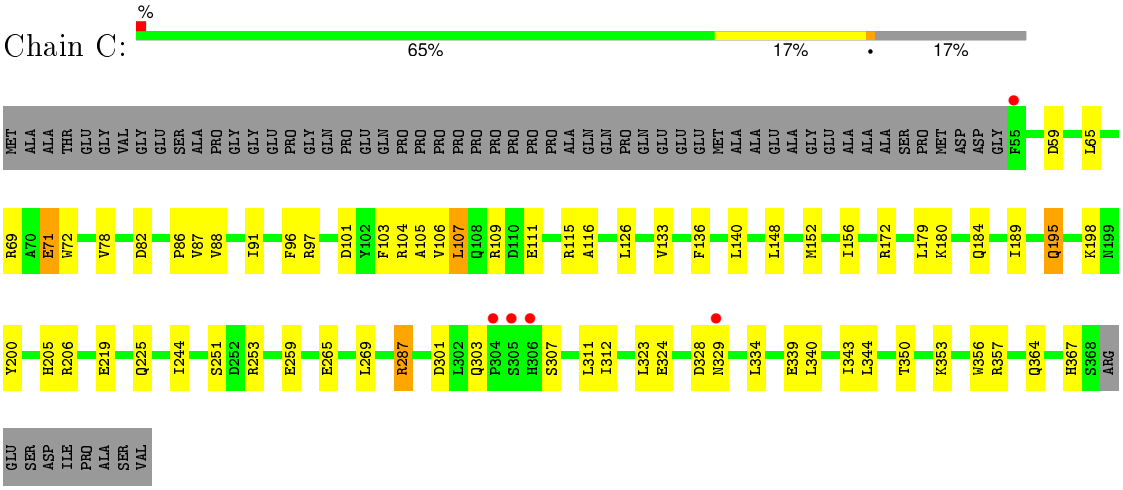
- Molecule 1: protein farnesyltransferase alpha subunit

Chain A:



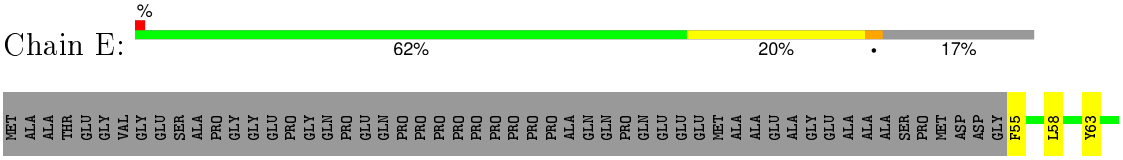
- Molecule 1: protein farnesyltransferase alpha subunit

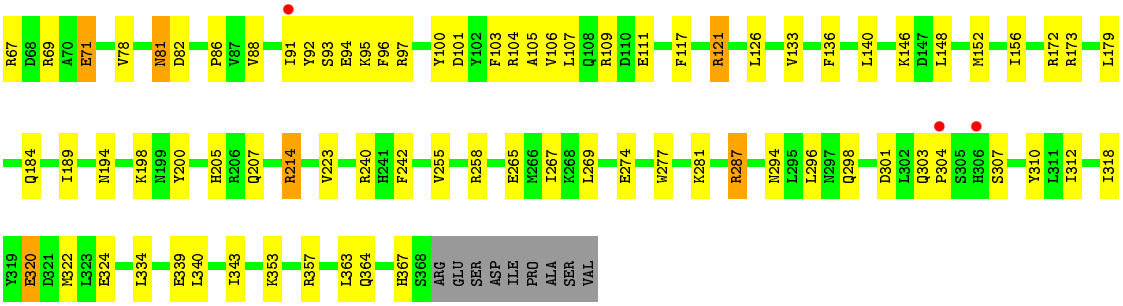
Chain C:



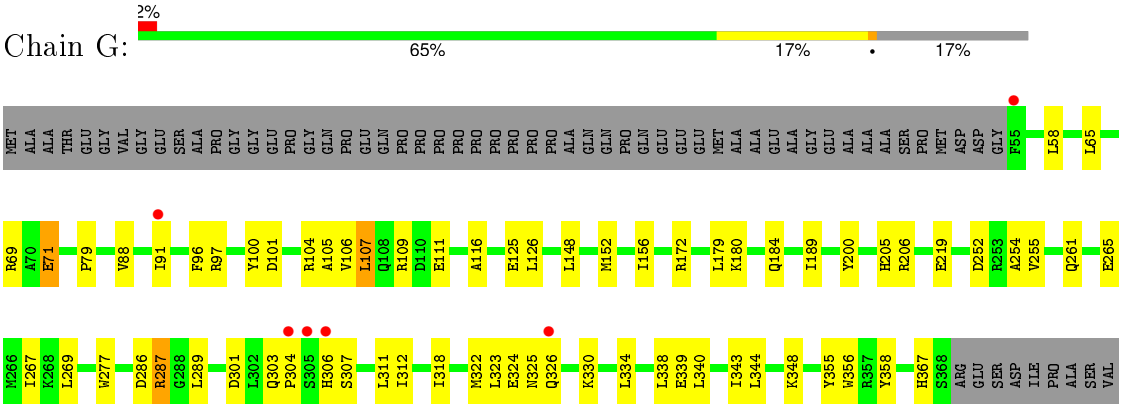
- Molecule 1: protein farnesyltransferase alpha subunit

Chain E:

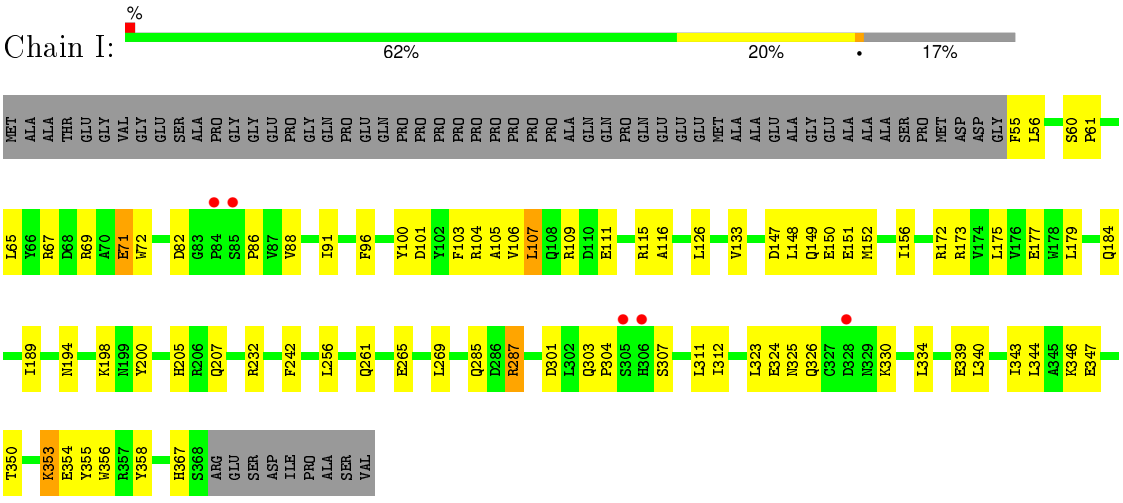




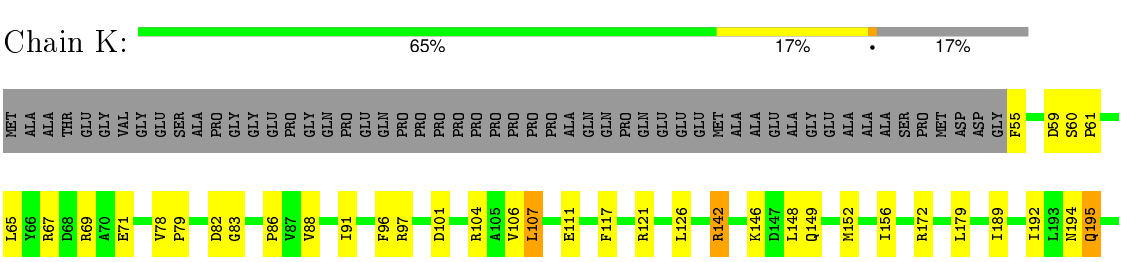
• Molecule 1: protein farnesyltransferase alpha subunit

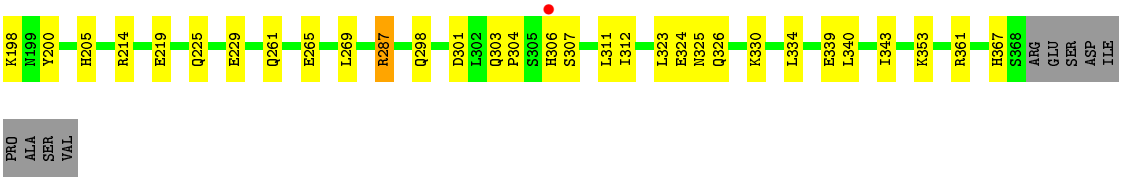


• Molecule 1: protein farnesyltransferase alpha subunit

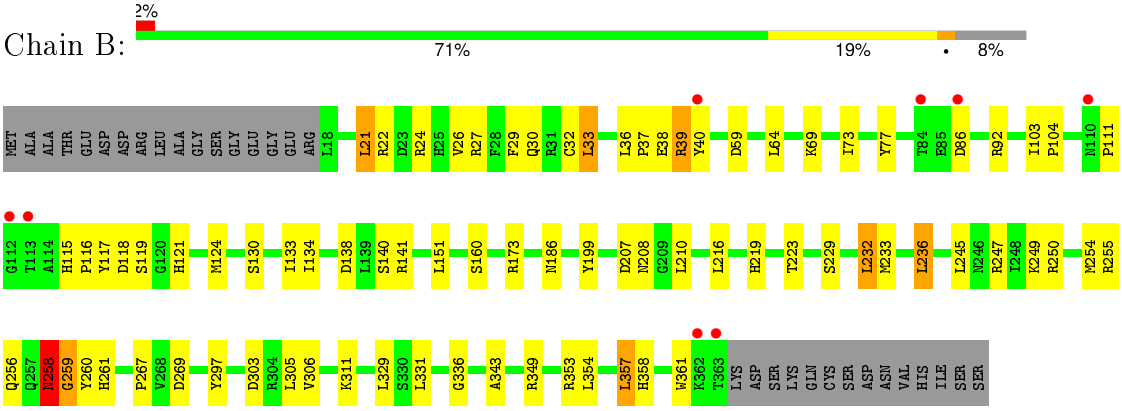


• Molecule 1: protein farnesyltransferase alpha subunit

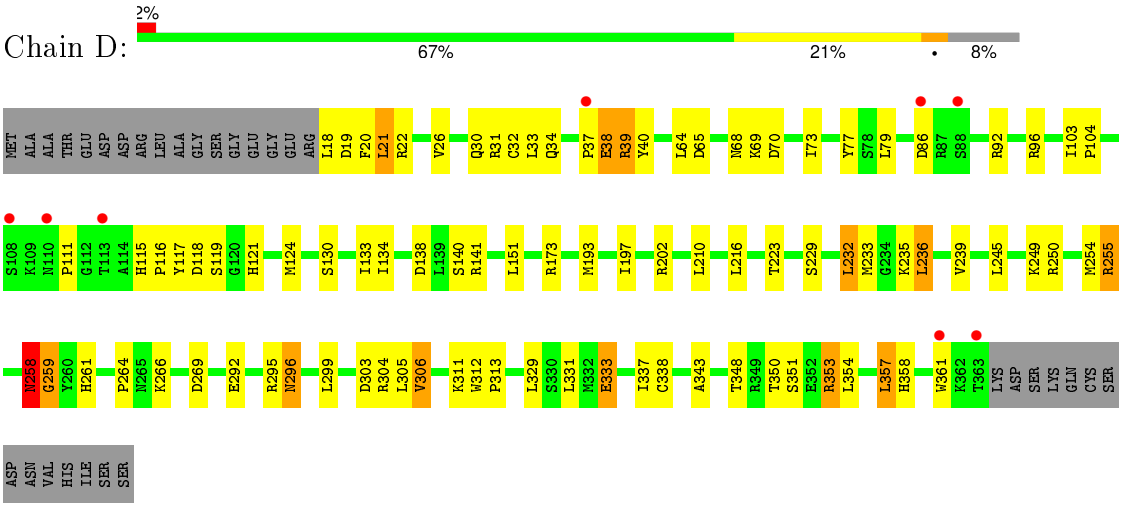




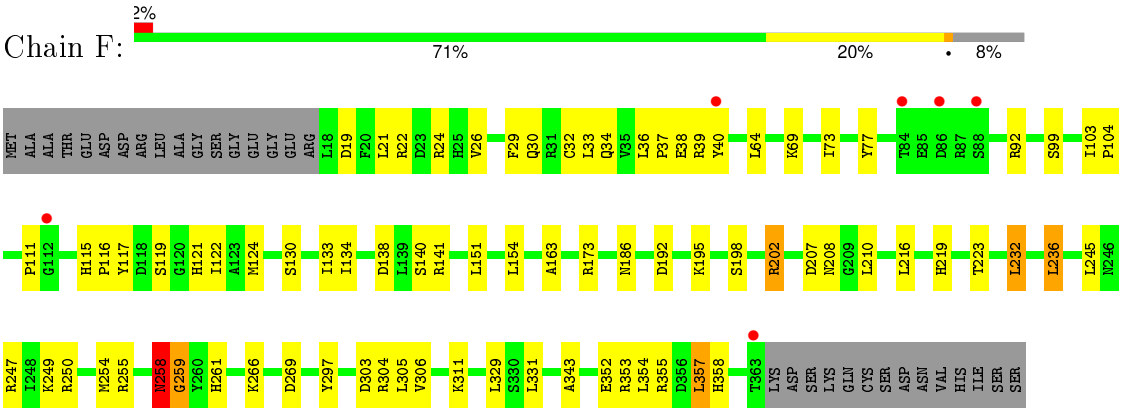
• Molecule 2: geranyltransferase type-I beta subunit



• Molecule 2: geranyltransferase type-I beta subunit

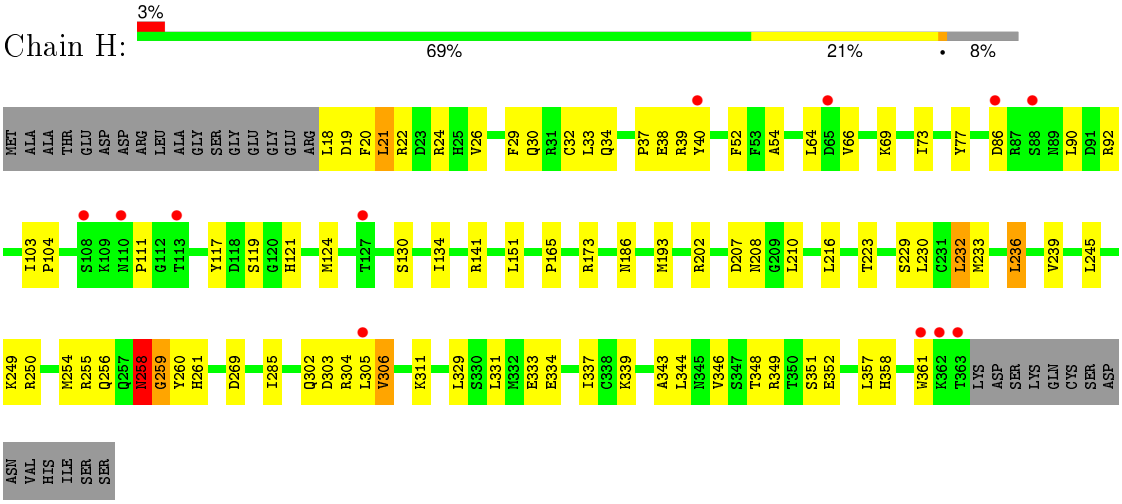


• Molecule 2: geranyltransferase type-I beta subunit



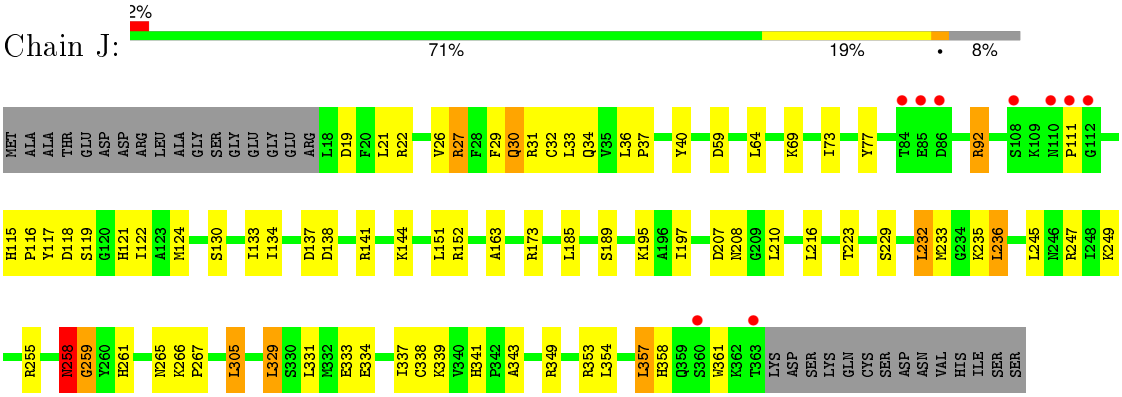
• Molecule 2: geranyltransferase type-I beta subunit

Chain H:



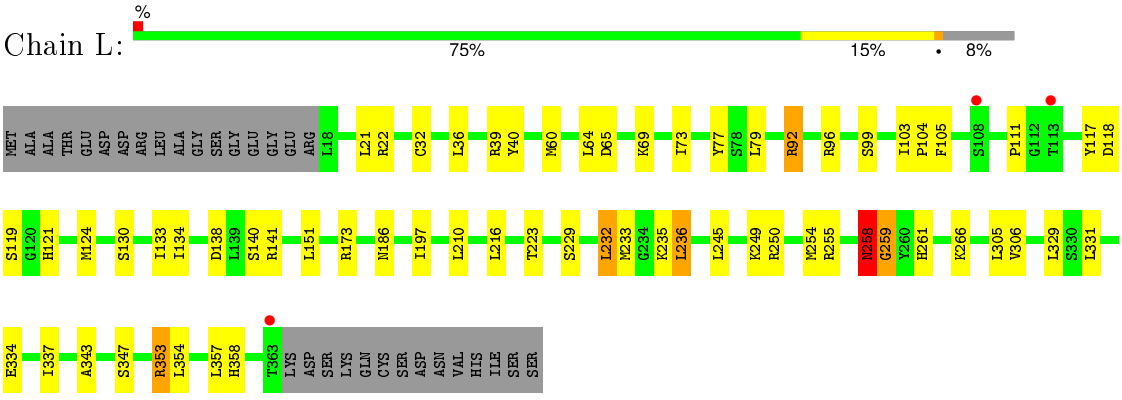
• Molecule 2: geranyltransferase type-I beta subunit

Chain J:



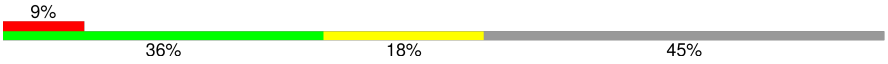
• Molecule 2: geranyltransferase type-I beta subunit

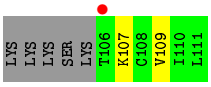
Chain L:



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

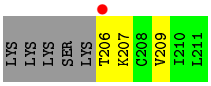
Chain M:





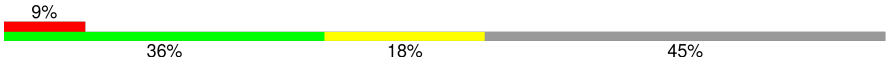
• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain N:



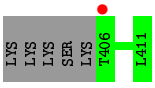
• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain O:



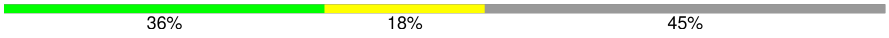
• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

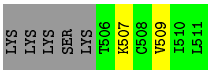
Chain P:



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

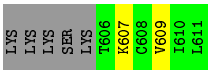
Chain Q:





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

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	272.07Å 268.80Å 185.31Å 90.00° 131.55° 90.00°	Depositor
Resolution (Å)	29.86 – 2.80 29.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.86-2.80) 95.3 (29.86-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.200 , 0.218 0.199 , 0.218	Depositor DCC
R_{free} test set	12101 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.6	EDS
Estimated twinning fraction	0.085 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 288709 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33129	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

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

[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: GER, ZN, SO4, MES, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/2680	0.52	0/3649
1	C	0.36	0/2714	0.53	0/3690
1	E	0.35	0/2696	0.53	0/3668
1	G	0.36	0/2698	0.53	0/3670
1	I	0.36	0/2720	0.54	0/3698
1	K	0.39	0/2733	0.56	0/3713
2	B	0.36	0/2750	0.60	2/3720 (0.1%)
2	D	0.37	0/2754	0.59	2/3725 (0.1%)
2	F	0.38	0/2769	0.60	2/3743 (0.1%)
2	H	0.35	0/2730	0.58	2/3696 (0.1%)
2	J	0.36	0/2770	0.59	2/3745 (0.1%)
2	L	0.39	0/2775	0.61	2/3750 (0.1%)
3	M	0.54	0/45	0.50	0/58
3	N	0.52	0/45	0.51	0/58
3	O	0.54	0/45	0.53	0/58
3	P	0.50	0/45	0.51	0/58
3	Q	0.55	0/45	0.52	0/58
3	R	0.56	0/45	0.53	0/58
All	All	0.37	0/33059	0.57	12/44815 (0.0%)

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

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	259	GLY	N-CA-C	-5.88	98.40	113.10
2	F	259	GLY	N-CA-C	-5.80	98.61	113.10
2	L	259	GLY	N-CA-C	-5.79	98.62	113.10
2	H	259	GLY	N-CA-C	-5.75	98.73	113.10
2	D	259	GLY	N-CA-C	-5.65	98.97	113.10
2	B	258	ASN	N-CA-C	-5.56	95.99	111.00
2	B	259	GLY	N-CA-C	-5.53	99.28	113.10
2	J	258	ASN	N-CA-C	-5.46	96.26	111.00
2	L	258	ASN	N-CA-C	-5.42	96.38	111.00
2	D	258	ASN	N-CA-C	-5.38	96.48	111.00
2	F	258	ASN	N-CA-C	-5.38	96.48	111.00
2	H	258	ASN	N-CA-C	-5.34	96.57	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	2614	0	2499	58	0
1	C	2648	0	2549	50	0
1	E	2630	0	2524	69	0
1	G	2632	0	2527	57	0
1	I	2654	0	2551	54	0
1	K	2667	0	2577	54	0
2	B	2689	0	2585	55	0
2	D	2693	0	2589	64	0
2	F	2708	0	2613	48	0
2	H	2670	0	2551	66	0
2	J	2709	0	2610	46	0
2	L	2714	0	2621	39	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	51	0	0	2	0
9	G	40	0	0	4	0
9	H	23	0	0	0	0
9	I	52	0	0	0	0
9	J	36	0	0	2	0
9	K	101	0	0	4	0
9	L	60	0	0	0	0
9	M	1	0	0	0	0
9	N	3	0	0	0	0
9	O	1	0	0	0	0
9	Q	3	0	0	0	0
9	R	5	0	0	0	0
All	All	33129	0	31390	639	0

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 10.

All (639) 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:E:156:ILE:HG12	1:E:172:ARG:HH12	1.12	1.14
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.14
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.12	1.12
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.15	1.11
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.16	1.09
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.26	0.97
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.83	0.94
7:G:804:CL:CL	9:G:913:HOH:O	2.23	0.92
1:E:81:ASN:N	1:E:81:ASN:HD22	1.70	0.89
1:C:353:LYS:HE2	1:C:357:ARG:HH12	1.38	0.86
1:E:81:ASN:HD22	1:E:81:ASN:H	1.25	0.84
2:H:21:LEU:HD22	2:H:302:GLN:HE21	1.41	0.82
2:H:21:LEU:HD13	2:H:302:GLN:HE22	1.42	0.82
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.44	0.82
2:D:69:LYS:O	2:D:73:ILE:HG13	1.82	0.79
2:H:348:THR:O	2:H:352:GLU:HG2	1.83	0.79
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.94	0.78
2:B:92:ARG:NH1	2:B:119:SER:HB3	2.00	0.76
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.51	0.76
2:F:69:LYS:O	2:F:73:ILE:HG13	1.86	0.76
1:C:353:LYS:HE2	1:C:357:ARG:NH1	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.68	0.75
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.21	0.75
1:A:152:MET:O	1:A:156:ILE:HG13	1.86	0.75
2:H:229:SER:O	2:H:233:MET:HG3	1.86	0.75
2:J:92:ARG:HH11	2:J:119:SER:HB3	1.52	0.74
1:G:152:MET:O	1:G:156:ILE:HG13	1.88	0.74
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.23	0.72
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.71	0.72
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.92	0.72
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.99	0.71
1:I:152:MET:O	1:I:156:ILE:HG13	1.90	0.71
7:K:807:CL:CL	9:K:986:HOH:O	2.46	0.71
2:B:69:LYS:O	2:B:73:ILE:HG13	1.89	0.71
2:J:92:ARG:NH1	2:J:119:SER:HB3	2.05	0.70
1:I:91:ILE:HD12	1:I:91:ILE:O	1.90	0.70
1:K:152:MET:O	1:K:156:ILE:HG13	1.91	0.70
1:E:152:MET:O	1:E:156:ILE:HG13	1.91	0.70
1:C:152:MET:O	1:C:156:ILE:HG13	1.90	0.70
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.56	0.70
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.97	0.69
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.27	0.69
2:H:21:LEU:HD13	2:H:302:GLN:NE2	2.07	0.68
2:H:69:LYS:O	2:H:73:ILE:HG13	1.92	0.68
7:G:804:CL:CL	9:G:932:HOH:O	2.47	0.68
1:A:339:GLU:O	1:A:343:ILE:HG13	1.93	0.68
1:E:105:ALA:O	1:E:109:ARG:HG3	1.94	0.68
7:C:801:CL:CL	9:C:922:HOH:O	2.47	0.68
1:C:323:LEU:HD13	1:C:367:HIS:HD2	1.60	0.67
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.29	0.67
1:A:91:ILE:O	1:A:91:ILE:HD12	1.94	0.67
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.60	0.67
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.77	0.67
1:E:81:ASN:N	1:E:81:ASN:ND2	2.42	0.67
2:H:349:ARG:O	2:H:352:GLU:HB2	1.94	0.67
1:E:91:ILE:O	1:E:91:ILE:HD12	1.95	0.67
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.30	0.65
1:K:91:ILE:O	1:K:91:ILE:HD12	1.97	0.65
2:B:92:ARG:HH11	2:B:119:SER:HB3	1.61	0.65
1:G:91:ILE:HD12	1:G:91:ILE:O	1.96	0.65
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.62	0.65
1:G:334:LEU:HD22	1:G:367:HIS:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.12	0.65
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.96	0.65
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.62	0.64
1:C:91:ILE:O	1:C:91:ILE:HD12	1.98	0.64
2:F:30:GLN:O	2:F:34:GLN:HG3	1.97	0.64
1:I:323:LEU:HB3	1:I:367:HIS:CD2	2.32	0.64
1:A:323:LEU:HB3	1:A:367:HIS:CD2	2.33	0.64
1:I:334:LEU:HD22	1:I:367:HIS:O	1.97	0.64
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.34	0.63
1:G:252:ASP:OD2	1:G:255:VAL:HG23	1.98	0.62
2:B:24:ARG:HD3	2:B:27:ARG:HH12	1.62	0.62
2:J:22:ARG:O	2:J:26:VAL:HG23	1.99	0.62
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.82	0.62
2:H:245:LEU:O	2:H:249:LYS:HG3	1.98	0.62
2:H:21:LEU:HD22	2:H:302:GLN:NE2	2.13	0.62
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.64	0.62
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.65	0.61
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.81	0.61
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.82	0.61
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.35	0.61
1:C:339:GLU:O	1:C:343:ILE:HG13	2.00	0.61
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.83	0.61
2:B:245:LEU:O	2:B:249:LYS:HG3	2.01	0.61
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.81	0.61
2:H:193:MET:HG3	2:H:233:MET:CE	2.31	0.61
1:E:320:GLU:OE2	1:E:363:LEU:HD21	2.01	0.61
2:H:26:VAL:O	2:H:30:GLN:HG3	2.01	0.61
2:J:358:HIS:O	2:J:361:TRP:HB2	2.01	0.61
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.82	0.60
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.01	0.60
2:D:229:SER:O	2:D:233:MET:HG3	2.01	0.60
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.81	0.60
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.67	0.60
2:H:193:MET:HG3	2:H:233:MET:HE1	1.83	0.60
1:C:323:LEU:HD13	1:C:367:HIS:CD2	2.35	0.60
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.82	0.60
2:F:26:VAL:O	2:F:30:GLN:HG3	2.01	0.60
2:L:69:LYS:O	2:L:73:ILE:HG13	2.02	0.60
1:I:100:TYR:O	1:I:104:ARG:HG3	2.00	0.60
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.36	0.60
1:E:214:ARG:O	1:E:214:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.37	0.60
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.66	0.60
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.65	0.60
1:G:330:LYS:HE2	1:G:367:HIS:HB3	1.84	0.59
1:I:207:GLN:HG2	1:I:242:PHE:CE2	2.37	0.59
2:L:245:LEU:O	2:L:249:LYS:HG3	2.03	0.59
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.83	0.59
2:J:69:LYS:O	2:J:73:ILE:HG13	2.02	0.59
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.01	0.59
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.16	0.59
2:J:92:ARG:NH1	2:J:118:ASP:O	2.33	0.59
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.08	0.59
1:E:78:VAL:O	1:E:104:ARG:HD2	2.02	0.59
2:F:303:ASP:OD1	2:F:306:VAL:HG13	2.03	0.58
2:H:18:LEU:N	2:H:18:LEU:HD22	2.17	0.58
2:H:303:ASP:OD1	2:H:306:VAL:HG13	2.03	0.58
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.68	0.58
1:E:67:ARG:NH2	1:E:94:GLU:OE1	2.36	0.58
1:I:261:GLN:O	1:I:265:GLU:HG2	2.04	0.58
1:I:105:ALA:O	1:I:109:ARG:HG3	2.03	0.58
1:G:339:GLU:O	1:G:343:ILE:HG13	2.03	0.58
1:C:328:ASP:O	1:C:329:ASN:HB2	2.03	0.58
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.85	0.58
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.86	0.58
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.86	0.58
1:G:261:GLN:O	1:G:265:GLU:HG2	2.04	0.57
2:D:173:ARG:HG2	8:N:1208:GER:H111	1.85	0.57
2:B:29:PHE:O	2:B:33:LEU:HD22	2.03	0.57
2:F:138:ASP:HA	2:F:357:LEU:HD11	1.85	0.57
1:A:334:LEU:HD22	1:A:367:HIS:O	2.03	0.57
2:F:173:ARG:HG2	8:O:1308:GER:H111	1.86	0.57
1:G:58:LEU:HD12	1:G:125:GLU:OE2	2.04	0.57
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.85	0.57
1:E:339:GLU:O	1:E:343:ILE:HG13	2.05	0.57
1:K:334:LEU:HD22	1:K:367:HIS:O	2.04	0.57
2:L:39:ARG:HG3	2:L:40:TYR:CE1	2.40	0.57
2:H:92:ARG:HG2	2:H:165:PRO:HG3	1.86	0.57
2:J:258:ASN:OD1	2:J:259:GLY:N	2.32	0.57
2:H:210:LEU:HB2	2:H:223:THR:HA	1.87	0.57
1:I:88:VAL:HG12	2:J:32:CYS:O	2.05	0.57
1:A:78:VAL:O	1:A:104:ARG:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.86	0.56
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.40	0.56
2:F:198:SER:O	2:F:202:ARG:HG3	2.05	0.56
1:K:301:ASP:O	1:K:304:PRO:HD2	2.06	0.56
2:D:333:GLU:HA	9:D:835:HOH:O	2.06	0.56
2:D:296:ASN:HD22	2:D:296:ASN:C	2.07	0.56
2:H:193:MET:HE2	2:H:233:MET:HB3	1.86	0.56
1:C:334:LEU:HD22	1:C:367:HIS:O	2.05	0.56
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.21	0.56
2:H:52:PHE:HE1	2:H:130:SER:HG	1.51	0.56
2:F:130:SER:O	2:F:134:ILE:HG13	2.06	0.56
2:J:210:LEU:HB2	2:J:223:THR:HA	1.87	0.56
2:B:258:ASN:OD1	2:B:259:GLY:N	2.38	0.56
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.41	0.56
1:I:200:TYR:HB3	4:I:905:MES:H32	1.88	0.56
2:J:173:ARG:HG2	8:Q:1508:GER:H111	1.88	0.56
2:D:303:ASP:OD1	2:D:306:VAL:HG13	2.05	0.56
2:L:210:LEU:HB2	2:L:223:THR:HA	1.87	0.56
1:E:121:ARG:HG3	1:E:121:ARG:NH1	2.19	0.56
2:J:195:LYS:NZ	9:J:840:HOH:O	2.38	0.56
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.88	0.55
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.72	0.55
2:B:26:VAL:O	2:B:30:GLN:HG3	2.06	0.55
2:B:173:ARG:HG2	8:M:1108:GER:H111	1.86	0.55
2:D:26:VAL:O	2:D:30:GLN:HG3	2.06	0.55
1:C:303:GLN:O	1:C:307:SER:HB2	2.07	0.55
2:L:186:ASN:HB2	2:L:358:HIS:NE2	2.21	0.55
2:B:39:ARG:HH11	2:B:39:ARG:CB	2.19	0.55
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.88	0.55
2:F:210:LEU:HB2	2:F:223:THR:HA	1.88	0.55
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.41	0.55
2:B:210:LEU:HB2	2:B:223:THR:HA	1.88	0.55
2:D:210:LEU:HB2	2:D:223:THR:HA	1.88	0.55
1:A:303:GLN:O	1:A:307:SER:HB2	2.07	0.55
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.42	0.55
2:H:258:ASN:OD1	2:H:259:GLY:N	2.36	0.55
2:D:202:ARG:HG3	2:D:202:ARG:HH11	1.71	0.55
1:I:156:ILE:CG1	1:I:172:ARG:HH12	2.05	0.55
2:H:173:ARG:HG2	8:P:1408:GER:H111	1.89	0.55
2:D:30:GLN:O	2:D:34:GLN:HG3	2.06	0.54
1:E:334:LEU:HD22	1:E:367:HIS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:GLN:NE2	1:K:179:LEU:HD13	2.23	0.54
1:G:100:TYR:O	1:G:104:ARG:HG3	2.06	0.54
1:K:198:LYS:HD3	2:L:266:LYS:HD3	1.89	0.54
2:D:121:HIS:HB3	2:D:124:MET:HG2	1.90	0.54
2:D:31:ARG:HH22	2:D:306:VAL:HG23	1.72	0.54
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.89	0.54
2:D:258:ASN:OD1	2:D:259:GLY:N	2.33	0.54
1:A:261:GLN:O	1:A:265:GLU:HG2	2.07	0.54
2:F:64:LEU:HD11	2:F:134:ILE:HG22	1.91	0.53
1:I:65:LEU:O	1:I:69:ARG:HG3	2.08	0.53
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.73	0.53
1:I:69:ARG:HB3	1:I:71:GLU:OE1	2.08	0.53
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.02	0.53
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.91	0.53
1:I:156:ILE:HG12	1:I:172:ARG:NH1	2.01	0.53
1:G:252:ASP:OD2	1:G:254:ALA:HB3	2.09	0.53
1:I:106:VAL:HG13	1:I:111:GLU:HB3	1.90	0.53
1:E:81:ASN:H	1:E:81:ASN:ND2	2.00	0.53
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.24	0.53
1:A:301:ASP:O	1:A:304:PRO:HD2	2.08	0.53
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.72	0.53
1:C:350:THR:O	1:C:353:LYS:HB2	2.08	0.53
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.44	0.53
1:E:58:LEU:HD22	1:E:95:LYS:HD3	1.90	0.53
2:D:19:ASP:OD2	2:D:19:ASP:N	2.42	0.53
1:K:323:LEU:HB3	1:K:367:HIS:CD2	2.44	0.53
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.44	0.53
1:E:121:ARG:HG3	1:E:121:ARG:HH11	1.74	0.53
2:H:130:SER:O	2:H:134:ILE:HG13	2.09	0.52
1:K:88:VAL:HG12	2:L:32:CYS:O	2.10	0.52
2:J:121:HIS:HB3	2:J:124:MET:HG2	1.91	0.52
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.08	0.52
1:C:311:LEU:HD23	1:C:311:LEU:C	2.30	0.52
2:F:121:HIS:HB3	2:F:124:MET:HG2	1.92	0.52
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.92	0.52
1:K:311:LEU:HD23	1:K:311:LEU:C	2.29	0.52
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.92	0.52
1:G:303:GLN:O	1:G:307:SER:HB2	2.10	0.52
1:G:334:LEU:O	1:G:338:LEU:HG	2.09	0.52
1:G:88:VAL:HG12	2:H:32:CYS:O	2.09	0.52
1:A:92:TYR:O	1:A:97:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:LEU:HD12	2:D:304:ARG:NH1	2.25	0.52
2:H:21:LEU:HD23	2:H:24:ARG:HD2	1.90	0.52
1:G:65:LEU:O	1:G:69:ARG:HG3	2.09	0.52
2:L:121:HIS:HB3	2:L:124:MET:HG2	1.92	0.52
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.09	0.52
2:L:173:ARG:HG2	8:R:1608:GER:H111	1.91	0.52
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.92	0.52
1:E:353:LYS:HE3	1:E:357:ARG:NH2	2.20	0.52
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.45	0.51
1:E:92:TYR:O	1:E:97:ARG:NH2	2.43	0.51
1:K:303:GLN:O	1:K:307:SER:HB2	2.11	0.51
2:J:130:SER:O	2:J:134:ILE:HG13	2.10	0.51
1:A:274:GLU:HG2	1:A:278:ASN:HD21	1.74	0.51
1:I:311:LEU:C	1:I:311:LEU:HD23	2.31	0.51
1:C:78:VAL:O	1:C:104:ARG:HD2	2.09	0.51
2:H:357:LEU:HD21	2:H:361:TRP:CZ2	2.45	0.51
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.90	0.51
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.93	0.51
1:I:200:TYR:CB	4:I:905:MES:H32	2.40	0.51
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.45	0.51
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.92	0.51
1:I:301:ASP:O	1:I:304:PRO:HD2	2.11	0.51
1:G:156:ILE:CG1	1:G:172:ARG:HH12	2.12	0.51
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.92	0.51
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.93	0.51
1:K:106:VAL:HG13	1:K:111:GLU:HB3	1.93	0.51
1:G:344:LEU:HA	1:G:348:LYS:HB2	1.92	0.51
1:A:214:ARG:O	1:A:214:ARG:HG3	2.11	0.51
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.92	0.51
2:F:103:ILE:HG23	2:F:104:PRO:HD2	1.92	0.51
1:C:88:VAL:HG12	2:D:32:CYS:O	2.10	0.51
1:A:184:GLN:HG3	9:A:907:HOH:O	2.11	0.51
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.93	0.51
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.91	0.51
1:E:93:SER:N	2:F:38:GLU:OE1	2.37	0.51
2:D:39:ARG:HG3	2:D:40:TYR:CE1	2.46	0.51
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.11	0.51
1:E:106:VAL:HG13	1:E:111:GLU:HB3	1.93	0.51
9:C:927:HOH:O	1:K:339:GLU:HA	2.10	0.51
2:H:121:HIS:HB3	2:H:124:MET:HG2	1.93	0.51
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ASP:HA	1:E:104:ARG:HH11	1.77	0.50
2:B:229:SER:O	2:B:233:MET:HG3	2.10	0.50
1:E:265:GLU:O	1:E:269:LEU:HD13	2.11	0.50
2:F:352:GLU:O	2:F:355:ARG:HB3	2.11	0.50
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.76	0.50
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.24	0.50
1:I:339:GLU:O	1:I:343:ILE:HG13	2.12	0.50
2:L:79:LEU:O	2:L:96:ARG:HG3	2.11	0.50
1:K:65:LEU:O	1:K:69:ARG:HG3	2.11	0.50
1:A:88:VAL:HG12	2:B:32:CYS:O	2.11	0.50
1:G:318:ILE:HG22	1:G:322:MET:HE2	1.93	0.50
2:B:207:ASP:O	2:B:208:ASN:HB2	2.12	0.50
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.47	0.50
1:K:311:LEU:HD23	1:K:311:LEU:O	2.12	0.50
2:B:121:HIS:HB3	2:B:124:MET:HG2	1.94	0.50
2:D:338:CYS:HB3	9:D:830:HOH:O	2.10	0.50
2:L:236:LEU:HD22	2:L:245:LEU:HD21	1.94	0.50
1:K:339:GLU:O	1:K:343:ILE:HG13	2.11	0.50
1:C:105:ALA:O	1:C:109:ARG:HG3	2.11	0.50
2:B:303:ASP:OD1	2:B:306:VAL:HG13	2.12	0.49
1:A:104:ARG:NH2	9:A:917:HOH:O	2.45	0.49
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.12	0.49
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.42	0.49
2:F:29:PHE:O	2:F:33:LEU:HD22	2.12	0.49
1:I:350:THR:O	1:I:353:LYS:HB3	2.12	0.49
1:G:105:ALA:O	1:G:109:ARG:HG3	2.12	0.49
1:A:106:VAL:HG13	1:A:111:GLU:HB3	1.94	0.49
1:E:173:ARG:NH1	9:E:921:HOH:O	2.41	0.49
1:G:311:LEU:HD23	1:G:311:LEU:C	2.32	0.49
1:E:274:GLU:HG3	1:E:310:TYR:CE2	2.48	0.49
1:I:330:LYS:HE2	1:I:367:HIS:HB3	1.94	0.49
1:K:330:LYS:HE2	1:K:367:HIS:HB3	1.94	0.49
1:G:106:VAL:HG13	1:G:111:GLU:HB3	1.93	0.49
1:G:200:TYR:HB3	4:G:904:MES:H32	1.95	0.49
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.85	0.49
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.94	0.49
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.47	0.49
1:G:340:LEU:HD23	1:G:343:ILE:HD12	1.94	0.49
1:C:148:LEU:CB	1:C:179:LEU:HD21	2.43	0.49
2:F:77:TYR:CE1	2:F:141:ARG:HB2	2.48	0.49
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.12	0.49
2:L:353:ARG:NH1	2:L:357:LEU:HG	2.28	0.49
1:E:100:TYR:O	1:E:104:ARG:HG3	2.12	0.49
2:F:99:SER:HB2	9:F:847:HOH:O	2.12	0.49
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.48	0.49
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.47	0.48
1:K:97:ARG:HG2	1:K:101:ASP:OD2	2.13	0.48
1:K:214:ARG:HH11	1:K:214:ARG:HG3	1.76	0.48
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.94	0.48
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.94	0.48
1:C:200:TYR:HB3	4:C:902:MES:H32	1.95	0.48
2:F:207:ASP:O	2:F:208:ASN:HB2	2.12	0.48
1:K:265:GLU:O	1:K:269:LEU:HD13	2.13	0.48
1:I:148:LEU:CB	1:I:179:LEU:HD21	2.43	0.48
1:G:148:LEU:CB	1:G:179:LEU:HD21	2.43	0.48
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.77	0.48
1:E:353:LYS:CE	1:E:357:ARG:HH12	2.25	0.48
1:A:214:ARG:CG	1:A:214:ARG:O	2.61	0.48
1:A:334:LEU:O	1:A:338:LEU:HG	2.13	0.48
1:A:161:GLU:HG3	1:A:162:GLN:HG3	1.96	0.48
2:D:130:SER:O	2:D:134:ILE:HG13	2.12	0.48
2:D:64:LEU:HD11	2:D:134:ILE:HG22	1.94	0.48
1:A:285:GLN:NE2	2:B:247:ARG:NH1	2.61	0.48
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.48	0.48
2:D:296:ASN:ND2	2:D:296:ASN:C	2.67	0.48
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.95	0.48
2:D:236:LEU:HD22	2:D:245:LEU:HD21	1.94	0.48
2:J:27:ARG:HH22	2:J:30:GLN:NE2	2.10	0.48
1:I:60:SER:OG	1:I:61:PRO:HD2	2.14	0.48
2:B:258:ASN:CG	2:B:259:GLY:H	2.16	0.48
2:B:130:SER:O	2:B:134:ILE:HG13	2.12	0.48
2:D:115:HIS:ND1	2:D:116:PRO:HD2	2.28	0.48
2:F:208:ASN:ND2	2:F:247:ARG:HB3	2.29	0.48
2:H:269:ASP:OD2	2:H:311:LYS:HE3	2.14	0.48
1:E:303:GLN:O	1:E:307:SER:HB2	2.13	0.48
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.95	0.48
2:L:92:ARG:NH1	2:L:118:ASP:O	2.47	0.48
1:E:207:GLN:HG2	1:E:242:PHE:CE2	2.49	0.48
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.94	0.48
2:H:186:ASN:HB2	2:H:358:HIS:NE2	2.28	0.48
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:GLU:HA	1:I:265:GLU:OE2	2.13	0.48
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.49	0.48
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.49	0.48
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.49	0.48
1:K:303:GLN:HB3	1:K:304:PRO:HD3	1.95	0.47
2:D:22:ARG:O	2:D:26:VAL:HG23	2.14	0.47
1:K:67:ARG:HD2	9:K:965:HOH:O	2.14	0.47
1:I:353:LYS:HG2	1:I:354:GLU:N	2.29	0.47
1:C:106:VAL:HG13	1:C:111:GLU:HB3	1.95	0.47
1:E:353:LYS:CE	1:E:357:ARG:HH22	2.22	0.47
1:E:148:LEU:CB	1:E:179:LEU:HD21	2.44	0.47
2:B:269:ASP:OD2	2:B:311:LYS:HE3	2.14	0.47
2:L:60:MET:HE2	2:L:347:SER:HB3	1.97	0.47
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.78	0.47
2:D:269:ASP:OD2	2:D:311:LYS:HE3	2.14	0.47
1:E:281:LYS:HD3	9:E:923:HOH:O	2.14	0.47
1:A:121:ARG:HD3	9:A:934:HOH:O	2.14	0.47
1:A:265:GLU:O	1:A:269:LEU:HD13	2.14	0.47
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.50	0.47
1:E:88:VAL:HG12	2:F:32:CYS:O	2.15	0.47
2:H:339:LYS:O	2:H:348:THR:HG23	2.14	0.47
1:K:82:ASP:OD2	2:L:99:SER:OG	2.33	0.47
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.97	0.47
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.96	0.47
1:E:301:ASP:O	1:E:304:PRO:HD2	2.15	0.47
1:I:232:ARG:HD3	2:J:265:ASN:ND2	2.28	0.47
2:B:37:PRO:HB2	2:B:39:ARG:HG2	1.97	0.47
2:B:64:LEU:HD11	2:B:134:ILE:HG22	1.96	0.47
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.50	0.47
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.15	0.47
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.48	0.46
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.78	0.46
2:B:236:LEU:HD22	2:B:245:LEU:HD21	1.97	0.46
2:J:30:GLN:HB3	2:J:30:GLN:HE21	1.62	0.46
2:D:312:TRP:HB3	2:D:313:PRO:HD2	1.97	0.46
2:B:357:LEU:HD22	2:B:361:TRP:CZ2	2.50	0.46
2:J:267:PRO:HG2	9:J:836:HOH:O	2.15	0.46
2:F:250:ARG:O	2:F:254:MET:HG2	2.14	0.46
1:K:200:TYR:HB3	4:K:906:MES:H32	1.97	0.46
2:H:22:ARG:O	2:H:26:VAL:HG23	2.15	0.46
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ILE:HD11	2:F:38:GLU:H	1.81	0.46
1:A:151:GLU:HG3	1:A:175:LEU:HD11	1.98	0.46
2:H:103:ILE:HG23	2:H:104:PRO:HD2	1.97	0.46
2:D:86:ASP:N	2:D:86:ASP:OD2	2.45	0.46
2:F:236:LEU:HD22	2:F:245:LEU:HD21	1.98	0.46
2:F:22:ARG:O	2:F:26:VAL:HG23	2.16	0.46
1:E:121:ARG:CG	1:E:121:ARG:HH11	2.29	0.46
2:J:333:GLU:OE1	2:J:339:LYS:HE3	2.15	0.46
1:E:296:LEU:HD22	1:E:322:MET:CE	2.46	0.46
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.51	0.46
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.46	0.46
1:K:214:ARG:HG3	1:K:214:ARG:NH1	2.31	0.46
2:J:152:ARG:HD3	2:J:189:SER:O	2.15	0.46
1:A:91:ILE:HD11	2:B:38:GLU:H	1.81	0.46
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.51	0.46
1:E:200:TYR:HB3	4:E:903:MES:H32	1.98	0.46
2:B:138:ASP:OD1	2:B:140:SER:HB3	2.16	0.45
2:F:192:ASP:CG	2:F:195:LYS:HG3	2.36	0.45
2:J:59:ASP:OD2	2:J:349:ARG:NH1	2.50	0.45
4:E:903:MES:H51	2:F:219:HIS:NE2	2.30	0.45
2:J:207:ASP:O	2:J:208:ASN:HB2	2.16	0.45
1:I:256:LEU:HD22	1:I:287:ARG:NH2	2.32	0.45
1:E:296:LEU:HD22	1:E:322:MET:HE3	1.97	0.45
1:A:355:TYR:O	1:A:358:TYR:HB3	2.17	0.45
2:H:18:LEU:N	2:H:18:LEU:CD2	2.80	0.45
2:H:20:PHE:CE2	2:H:337:ILE:HD11	2.52	0.45
2:J:245:LEU:O	2:J:249:LYS:HG3	2.17	0.45
2:B:92:ARG:NH1	2:B:118:ASP:O	2.50	0.45
2:D:354:LEU:HD11	2:D:358:HIS:HE2	1.80	0.45
1:C:340:LEU:HD23	1:C:343:ILE:HD12	1.98	0.45
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.99	0.45
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.52	0.45
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.17	0.45
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.31	0.45
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.50	0.45
2:D:236:LEU:CD2	2:D:245:LEU:HD21	2.47	0.45
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.52	0.45
2:H:37:PRO:HD2	2:H:40:TYR:CD1	2.52	0.45
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.31	0.45
1:E:318:ILE:HG22	1:E:322:MET:CE	2.47	0.45
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:LYS:O	1:I:347:GLU:HG2	2.16	0.45
1:C:344:LEU:HD13	1:C:356:TRP:CE2	2.52	0.45
2:J:19:ASP:OD2	2:J:19:ASP:N	2.48	0.45
2:F:154:LEU:HD11	9:F:827:HOH:O	2.16	0.45
2:H:30:GLN:O	2:H:34:GLN:HG3	2.17	0.45
2:B:250:ARG:O	2:B:254:MET:HG2	2.17	0.45
1:I:355:TYR:O	1:I:358:TYR:HB3	2.16	0.45
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.81	0.45
1:G:265:GLU:O	1:G:269:LEU:HD13	2.17	0.44
1:C:265:GLU:O	1:C:269:LEU:HD13	2.17	0.44
2:B:21:LEU:CD1	2:B:21:LEU:N	2.80	0.44
1:C:103:PHE:CZ	1:C:133:VAL:HG22	2.52	0.44
2:J:236:LEU:HD22	2:J:245:LEU:HD21	1.99	0.44
2:J:229:SER:O	2:J:233:MET:HG3	2.18	0.44
2:D:92:ARG:NH1	2:D:118:ASP:O	2.50	0.44
1:C:91:ILE:HD11	2:D:38:GLU:H	1.82	0.44
2:D:245:LEU:O	2:D:249:LYS:HG3	2.17	0.44
2:F:245:LEU:O	2:F:249:LYS:HG3	2.16	0.44
2:D:250:ARG:O	2:D:254:MET:HG2	2.18	0.44
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.32	0.44
2:D:92:ARG:HB3	2:D:119:SER:CB	2.48	0.44
2:B:59:ASP:OD2	2:B:349:ARG:NH1	2.49	0.44
2:H:29:PHE:O	2:H:33:LEU:HD22	2.18	0.44
1:K:325:ASN:O	1:K:326:GLN:C	2.55	0.44
2:L:130:SER:O	2:L:134:ILE:HG13	2.17	0.44
2:H:21:LEU:CD1	2:H:21:LEU:N	2.80	0.44
2:H:236:LEU:HD22	2:H:245:LEU:HD21	1.98	0.44
2:D:193:MET:HG3	2:D:233:MET:CE	2.47	0.44
1:E:214:ARG:O	1:E:214:ARG:CG	2.64	0.44
2:H:357:LEU:CD2	2:H:361:TRP:CZ2	3.01	0.44
1:I:147:ASP:OD1	1:I:150:GLU:N	2.48	0.44
1:I:173:ARG:O	1:I:177:GLU:HG3	2.16	0.44
1:C:353:LYS:CE	1:C:357:ARG:NH1	2.78	0.44
2:B:103:ILE:HG23	2:B:104:PRO:HD2	1.98	0.44
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.83	0.44
2:D:357:LEU:HD22	2:D:361:TRP:CZ2	2.53	0.44
1:K:65:LEU:HD12	1:K:67:ARG:NH1	2.33	0.44
1:I:303:GLN:O	1:I:307:SER:HB2	2.18	0.44
1:I:96:PHE:CE1	1:I:126:LEU:HB3	2.53	0.44
1:I:151:GLU:HG3	1:I:175:LEU:HD11	1.98	0.44
1:G:97:ARG:NH1	1:G:97:ARG:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:ILE:HG22	1:G:322:MET:CE	2.47	0.44
1:K:79:PRO:HA	1:K:101:ASP:OD1	2.18	0.44
2:H:348:THR:HA	2:H:351:SER:OG	2.17	0.44
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.53	0.44
1:C:219:GLU:OE1	1:C:219:GLU:HA	2.18	0.44
2:L:250:ARG:O	2:L:254:MET:HG2	2.18	0.44
1:E:357:ARG:HH11	1:E:357:ARG:HG3	1.83	0.43
1:I:265:GLU:O	1:I:269:LEU:HD13	2.19	0.43
1:I:103:PHE:CZ	1:I:133:VAL:HG22	2.53	0.43
1:C:195:GLN:H	1:C:195:GLN:HG2	1.58	0.43
1:C:65:LEU:O	1:C:69:ARG:HG3	2.18	0.43
4:A:901:MES:H51	2:B:219:HIS:NE2	2.34	0.43
1:G:267:ILE:HD13	1:G:277:TRP:CE2	2.53	0.43
1:C:253:ARG:HD3	1:I:56:LEU:HD22	2.00	0.43
1:I:198:LYS:HD3	2:J:266:LYS:HD3	1.99	0.43
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.53	0.43
2:D:77:TYR:CE1	2:D:141:ARG:HB2	2.53	0.43
1:I:287:ARG:H	1:I:287:ARG:HG2	1.56	0.43
1:C:287:ARG:H	1:C:287:ARG:HG2	1.62	0.43
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.53	0.43
1:E:294:ASN:O	1:E:298:GLN:HG3	2.19	0.43
1:I:325:ASN:O	1:I:326:GLN:C	2.57	0.43
1:G:286:ASP:HB2	9:G:941:HOH:O	2.17	0.43
2:J:77:TYR:HE2	2:J:137:ASP:OD2	2.01	0.43
1:A:311:LEU:HD23	1:A:311:LEU:C	2.39	0.43
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.47	0.43
1:K:149:GLN:HE22	1:K:179:LEU:HD13	1.84	0.43
1:K:261:GLN:O	1:K:265:GLU:HG2	2.18	0.43
2:F:92:ARG:HB3	2:F:119:SER:CB	2.48	0.43
2:H:24:ARG:NE	2:H:304:ARG:O	2.52	0.43
2:F:36:LEU:HA	2:F:37:PRO:HD3	1.86	0.43
2:L:77:TYR:CE1	2:L:141:ARG:HB2	2.54	0.43
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.49	0.43
3:N:206:THR:HB	3:N:207:LYS:H	1.68	0.43
2:H:19:ASP:O	2:H:21:LEU:HD13	2.19	0.43
2:D:354:LEU:HD11	2:D:358:HIS:NE2	2.33	0.43
2:H:258:ASN:CG	2:H:259:GLY:H	2.21	0.43
2:B:267:PRO:HG2	9:B:843:HOH:O	2.18	0.43
1:A:212:GLU:O	1:G:180:LYS:HE3	2.19	0.42
2:H:344:LEU:HB3	2:H:346:VAL:HG22	2.00	0.42
1:K:78:VAL:O	1:K:104:ARG:HD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:HB3	4:A:901:MES:H32	2.01	0.42
2:J:115:HIS:HA	2:J:116:PRO:HD3	1.91	0.42
2:J:29:PHE:O	2:J:33:LEU:HD22	2.18	0.42
2:L:229:SER:O	2:L:233:MET:HG3	2.19	0.42
1:K:219:GLU:OE1	1:K:219:GLU:HA	2.19	0.42
1:I:72:TRP:CZ2	1:I:115:ARG:HB2	2.53	0.42
1:G:91:ILE:HD11	2:H:38:GLU:H	1.83	0.42
1:E:318:ILE:HG22	1:E:322:MET:HE3	2.02	0.42
2:H:90:LEU:HD23	2:H:90:LEU:HA	1.91	0.42
1:G:323:LEU:HB3	1:G:367:HIS:CD2	2.54	0.42
1:I:149:GLN:NE2	1:I:179:LEU:HD13	2.34	0.42
2:H:33:LEU:HD22	2:H:54:ALA:HB1	2.00	0.42
1:C:136:PHE:CE2	1:C:140:LEU:HD11	2.54	0.42
2:J:144:LYS:HG2	2:J:185:LEU:HD22	2.01	0.42
2:L:258:ASN:OD1	2:L:259:GLY:N	2.45	0.42
2:F:122:ILE:HG22	2:F:163:ALA:HA	2.01	0.42
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.84	0.42
2:B:39:ARG:HG3	2:B:40:TYR:CE1	2.54	0.42
1:G:189:ILE:HG21	1:G:206:ARG:HB2	2.02	0.42
1:I:106:VAL:HG11	1:I:116:ALA:CB	2.50	0.42
2:L:173:ARG:HD2	8:R:1608:GER:H142	2.02	0.42
2:D:92:ARG:HH11	2:D:119:SER:HB3	1.85	0.42
2:D:68:ASN:OD1	2:D:70:ASP:HB2	2.19	0.42
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.55	0.42
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.47	0.42
2:D:37:PRO:O	2:D:39:ARG:N	2.53	0.42
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.01	0.42
1:C:244:ILE:HD11	1:C:259:GLU:OE1	2.20	0.42
1:E:287:ARG:H	1:E:287:ARG:HG2	1.48	0.42
2:J:329:LEU:HD12	2:J:329:LEU:HA	1.90	0.42
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.55	0.42
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.55	0.42
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.54	0.42
1:A:325:ASN:O	1:A:326:GLN:C	2.58	0.42
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.20	0.42
1:G:289:LEU:HG	9:G:936:HOH:O	2.19	0.42
2:H:86:ASP:N	2:H:86:ASP:OD2	2.48	0.42
2:B:86:ASP:N	2:B:86:ASP:OD2	2.47	0.42
2:B:64:LEU:HD23	2:B:64:LEU:HA	1.81	0.42
2:H:40:TYR:CD1	2:H:40:TYR:N	2.88	0.42
3:N:207:LYS:HE3	3:N:209:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:250:ARG:O	2:H:254:MET:HG2	2.20	0.42
3:R:607:LYS:HE3	3:R:609:VAL:HG22	2.01	0.42
3:M:107:LYS:HE3	3:M:109:VAL:HG22	2.02	0.42
2:H:207:ASP:O	2:H:208:ASN:HB2	2.20	0.42
2:L:92:ARG:HB3	2:L:119:SER:CB	2.49	0.41
2:H:37:PRO:HD2	2:H:40:TYR:CE1	2.55	0.41
1:I:82:ASP:HB2	1:I:86:PRO:HB3	2.01	0.41
2:B:160:SER:HB3	2:B:199:TYR:CE1	2.56	0.41
1:A:71:GLU:CD	1:A:71:GLU:H	2.15	0.41
1:K:353:LYS:HB2	1:K:353:LYS:HE3	1.70	0.41
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.79	0.41
2:F:258:ASN:CG	2:F:259:GLY:H	2.22	0.41
1:A:312:ILE:O	1:A:316:VAL:HG23	2.20	0.41
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.55	0.41
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.55	0.41
2:D:255:ARG:CZ	2:D:264:PRO:HG3	2.50	0.41
2:J:36:LEU:HA	2:J:37:PRO:HD3	1.91	0.41
1:C:87:VAL:CG1	2:D:33:LEU:HD12	2.51	0.41
1:A:105:ALA:O	1:A:109:ARG:HG3	2.21	0.41
2:J:122:ILE:HG22	2:J:163:ALA:HA	2.01	0.41
1:K:142:ARG:HA	1:K:142:ARG:HD3	1.83	0.41
1:K:361:ARG:HG3	9:K:947:HOH:O	2.20	0.41
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.85	0.41
2:F:37:PRO:C	2:F:39:ARG:H	2.24	0.41
1:A:189:ILE:HG21	1:A:206:ARG:HB2	2.03	0.41
1:A:66:TYR:CE1	1:A:119:LEU:HD13	2.55	0.41
2:F:37:PRO:C	2:F:39:ARG:N	2.73	0.41
2:B:186:ASN:HB2	2:B:358:HIS:NE2	2.34	0.41
1:K:101:ASP:HA	1:K:104:ARG:HH11	1.86	0.41
2:D:92:ARG:NH1	2:D:119:SER:HB3	2.36	0.41
1:A:308:SER:O	1:A:312:ILE:HG12	2.21	0.41
1:A:148:LEU:CB	1:A:179:LEU:HD21	2.47	0.41
1:I:106:VAL:HG11	1:I:116:ALA:HB1	2.03	0.41
2:D:19:ASP:O	2:D:21:LEU:HD13	2.20	0.41
2:H:37:PRO:C	2:H:39:ARG:N	2.74	0.41
2:L:22:ARG:HG2	2:L:22:ARG:NH1	2.35	0.41
1:K:225:GLN:NE2	1:K:229:GLU:OE2	2.52	0.41
2:B:115:HIS:HA	2:B:116:PRO:HD3	1.87	0.41
1:C:106:VAL:HG11	1:C:116:ALA:HB1	2.03	0.41
4:A:901:MES:H82	4:A:901:MES:H31	1.92	0.41
1:E:223:VAL:HG11	1:E:240:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:236:LEU:CD2	2:L:245:LEU:HD21	2.51	0.41
1:K:148:LEU:CB	1:K:179:LEU:HD21	2.49	0.41
1:G:106:VAL:HG11	1:G:116:ALA:HB1	2.03	0.41
4:G:904:MES:H31	4:G:904:MES:H82	1.94	0.41
2:D:235:LYS:O	2:D:239:VAL:HG23	2.21	0.41
1:G:355:TYR:O	1:G:358:TYR:HB3	2.21	0.41
3:Q:507:LYS:HE3	3:Q:509:VAL:HG22	2.03	0.41
1:G:287:ARG:HG2	1:G:287:ARG:H	1.56	0.41
1:A:192:ILE:O	1:A:195:GLN:HG3	2.21	0.41
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.21	0.41
1:I:285:GLN:NE2	2:J:247:ARG:NH1	2.68	0.41
1:C:189:ILE:HG21	1:C:206:ARG:HB2	2.03	0.41
1:K:91:ILE:HG13	2:L:36:LEU:O	2.21	0.41
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.86	0.41
1:C:251:SER:HA	1:C:287:ARG:HH12	1.86	0.41
2:H:230:LEU:HD22	2:H:239:VAL:HG21	2.03	0.41
2:L:197:ILE:HD11	2:L:235:LYS:HD3	2.02	0.41
2:L:64:LEU:HD23	2:L:64:LEU:HA	1.86	0.41
2:B:36:LEU:HA	2:B:37:PRO:HD3	1.83	0.40
2:B:232:LEU:HD13	2:B:343:ALA:HB1	2.03	0.40
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.92	0.40
1:E:136:PHE:CE2	1:E:140:LEU:HD11	2.56	0.40
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.56	0.40
2:J:64:LEU:HA	2:J:64:LEU:HD23	1.88	0.40
1:G:301:ASP:O	1:G:304:PRO:HD2	2.20	0.40
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.51	0.40
2:D:202:ARG:HH11	2:D:202:ARG:CG	2.34	0.40
3:O:307:LYS:HE3	3:O:309:VAL:HG22	2.02	0.40
1:E:267:ILE:HD13	1:E:277:TRP:CE2	2.56	0.40
1:A:274:GLU:HG2	1:A:278:ASN:ND2	2.36	0.40
1:C:72:TRP:CZ2	1:C:115:ARG:HB2	2.55	0.40
2:F:269:ASP:OD2	2:F:311:LYS:HE3	2.21	0.40
2:D:79:LEU:O	2:D:96:ARG:HG3	2.21	0.40
2:D:348:THR:HA	2:D:351:SER:OG	2.21	0.40
2:B:236:LEU:CD2	2:B:245:LEU:HD21	2.51	0.40
1:K:192:ILE:O	1:K:195:GLN:HG3	2.21	0.40
2:L:306:VAL:HG23	2:L:306:VAL:O	2.20	0.40
1:G:325:ASN:O	1:G:326:GLN:C	2.59	0.40
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.35	0.40
2:D:292:GLU:HG3	9:K:989:HOH:O	2.22	0.40
1:K:60:SER:OG	1:K:61:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:138:ASP:OD1	2:L:140:SER:HB3	2.21	0.40
1:K:287:ARG:HG2	1:K:287:ARG:H	1.60	0.40
2:F:19:ASP:OD2	2:F:304:ARG:NH2	2.54	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%)	288 (92%)	23 (7%)	1 (0%)	46 79
1	C	312/377 (83%)	292 (94%)	20 (6%)	0	100 100
1	E	312/377 (83%)	291 (93%)	21 (7%)	0	100 100
1	G	312/377 (83%)	287 (92%)	24 (8%)	1 (0%)	46 79
1	I	312/377 (83%)	290 (93%)	22 (7%)	0	100 100
1	K	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	46 79
2	B	344/377 (91%)	324 (94%)	18 (5%)	2 (1%)	30 65
2	D	344/377 (91%)	326 (95%)	14 (4%)	4 (1%)	16 47
2	F	344/377 (91%)	323 (94%)	19 (6%)	2 (1%)	30 65
2	H	344/377 (91%)	318 (92%)	22 (6%)	4 (1%)	16 47
2	J	344/377 (91%)	324 (94%)	17 (5%)	3 (1%)	21 55
2	L	344/377 (91%)	325 (94%)	17 (5%)	2 (1%)	30 65
3	M	4/11 (36%)	4 (100%)	0	0	100 100
3	N	4/11 (36%)	4 (100%)	0	0	100 100
3	O	4/11 (36%)	4 (100%)	0	0	100 100
3	P	4/11 (36%)	4 (100%)	0	0	100 100
3	Q	4/11 (36%)	4 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	R	4/11 (36%)	4 (100%)	0	0	100 100
All	All	3960/4590 (86%)	3704 (94%)	236 (6%)	20 (0%)	34 69

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	111	PRO
2	B	258	ASN
2	D	111	PRO
2	D	258	ASN
2	F	111	PRO
2	F	258	ASN
2	H	111	PRO
2	H	258	ASN
2	J	111	PRO
2	J	258	ASN
1	K	306	HIS
2	L	111	PRO
2	L	258	ASN
2	D	38	GLU
2	H	333	GLU
2	J	34	GLN
1	A	306	HIS
2	D	333	GLU
1	G	306	HIS
2	H	66	VAL

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	276/338 (82%)	270 (98%)	6 (2%)	60 89
1	C	285/338 (84%)	275 (96%)	10 (4%)	43 77
1	E	280/338 (83%)	269 (96%)	11 (4%)	39 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	281/338 (83%)	276 (98%)	5 (2%)	66 91
1	I	287/338 (85%)	278 (97%)	9 (3%)	47 81
1	K	290/338 (86%)	279 (96%)	11 (4%)	40 74
2	B	286/326 (88%)	273 (96%)	13 (4%)	34 68
2	D	287/326 (88%)	270 (94%)	17 (6%)	24 57
2	F	291/326 (89%)	276 (95%)	15 (5%)	29 62
2	H	282/326 (86%)	271 (96%)	11 (4%)	39 74
2	J	291/326 (89%)	274 (94%)	17 (6%)	25 57
2	L	292/326 (90%)	279 (96%)	13 (4%)	34 68
3	M	6/11 (54%)	6 (100%)	0	100 100
3	N	6/11 (54%)	6 (100%)	0	100 100
3	O	6/11 (54%)	6 (100%)	0	100 100
3	P	6/11 (54%)	6 (100%)	0	100 100
3	Q	6/11 (54%)	6 (100%)	0	100 100
3	R	6/11 (54%)	6 (100%)	0	100 100
All	All	3464/4050 (86%)	3326 (96%)	138 (4%)	38 73

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	71	GLU
1	A	184	GLN
1	A	195	GLN
1	A	214	ARG
1	A	287	ARG
2	B	21	LEU
2	B	33	LEU
2	B	39	ARG
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU
2	B	255	ARG
2	B	261	HIS
2	B	305	LEU
2	B	329	LEU

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Mol	Chain	Res	Type
2	B	331	LEU
2	B	357	LEU
1	C	59	ASP
1	C	71	GLU
1	C	107	LEU
1	C	184	GLN
1	C	195	GLN
1	C	225	GLN
1	C	287	ARG
1	C	301	ASP
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	39	ARG
2	D	65	ASP
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	296	ASN
2	D	305	LEU
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
2	D	353	ARG
2	D	357	LEU
1	E	55	PHE
1	E	71	GLU
1	E	81	ASN
1	E	121	ARG
1	E	184	GLN
1	E	194	ASN
1	E	214	ARG
1	E	287	ARG
1	E	320	GLU
1	E	324	GLU
1	E	364	GLN
2	F	21	LEU
2	F	24	ARG

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Mol	Chain	Res	Type
2	F	151	LEU
2	F	202	ARG
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	305	LEU
2	F	329	LEU
2	F	331	LEU
2	F	353	ARG
2	F	357	LEU
1	G	71	GLU
1	G	107	LEU
1	G	184	GLN
1	G	287	ARG
1	G	324	GLU
2	H	21	LEU
2	H	151	LEU
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	255	ARG
2	H	261	HIS
2	H	305	LEU
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
1	I	55	PHE
1	I	67	ARG
1	I	71	GLU
1	I	107	LEU
1	I	184	GLN
1	I	194	ASN
1	I	287	ARG
1	I	324	GLU
1	I	353	LYS
2	J	21	LEU
2	J	27	ARG
2	J	30	GLN
2	J	31	ARG

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Mol	Chain	Res	Type
2	J	92	ARG
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	305	LEU
2	J	329	LEU
2	J	331	LEU
2	J	341	HIS
2	J	353	ARG
2	J	357	LEU
1	K	55	PHE
1	K	59	ASP
1	K	71	GLU
1	K	107	LEU
1	K	121	ARG
1	K	142	ARG
1	K	194	ASN
1	K	195	GLN
1	K	287	ARG
1	K	298	GLN
1	K	324	GLU
2	L	21	LEU
2	L	65	ASP
2	L	92	ARG
2	L	151	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	255	ARG
2	L	261	HIS
2	L	305	LEU
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 (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN

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Mol	Chain	Res	Type
1	A	278	ASN
1	A	285	GLN
1	A	367	HIS
2	B	208	ASN
2	B	265	ASN
1	C	81	ASN
1	C	108	GLN
1	C	170	HIS
1	C	184	GLN
1	C	195	GLN
1	C	201	HIS
1	C	225	GLN
1	C	298	GLN
1	C	364	GLN
1	C	367	HIS
2	D	246	ASN
2	D	265	ASN
2	D	296	ASN
1	E	81	ASN
1	E	89	GLN
1	E	184	GLN
1	E	367	HIS
2	F	30	GLN
2	F	246	ASN
2	F	265	ASN
1	G	80	GLN
1	G	81	ASN
1	G	89	GLN
1	G	162	GLN
1	G	184	GLN
1	G	297	ASN
2	H	246	ASN
2	H	265	ASN
2	H	302	GLN
1	I	81	ASN
1	I	89	GLN
1	I	149	GLN
1	I	184	GLN
1	I	195	GLN
1	I	285	GLN
1	I	364	GLN
2	J	30	GLN

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Mol	Chain	Res	Type
2	J	34	GLN
2	J	208	ASN
2	J	246	ASN
2	J	265	ASN
1	K	149	GLN
1	K	184	GLN
1	K	297	ASN
1	K	298	GLN
2	L	246	ASN
2	L	265	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MES	A	901	-	11,12,12	6.39	7 (63%)	14,16,16	3.10	6 (42%)
6	SO4	B	810	-	4,4,4	0.11	0	6,6,6	0.11	0
4	MES	C	902	-	11,12,12	6.35	7 (63%)	14,16,16	3.16	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	D	811	-	4,4,4	0.12	0	6,6,6	0.15	0
4	MES	E	903	-	11,12,12	6.38	7 (63%)	14,16,16	3.10	6 (42%)
6	SO4	F	812	-	4,4,4	0.20	0	6,6,6	0.12	0
4	MES	G	904	-	11,12,12	6.34	7 (63%)	14,16,16	3.10	6 (42%)
6	SO4	H	813	-	4,4,4	0.14	0	6,6,6	0.20	0
4	MES	I	905	-	11,12,12	6.29	7 (63%)	14,16,16	3.28	6 (42%)
6	SO4	J	814	-	4,4,4	0.15	0	6,6,6	0.21	0
4	MES	K	906	-	11,12,12	6.21	7 (63%)	14,16,16	3.29	6 (42%)
6	SO4	L	815	-	4,4,4	0.10	0	6,6,6	0.27	0
8	GER	M	1108	3	19,19,19	0.82	0	22,22,22	0.77	0
8	GER	N	1208	3	19,19,19	0.75	0	22,22,22	0.77	0
8	GER	O	1308	3	19,19,19	0.78	0	22,22,22	0.79	0
8	GER	P	1408	3	19,19,19	0.71	0	22,22,22	0.78	0
8	GER	Q	1508	3	19,19,19	0.76	0	22,22,22	0.79	0
8	GER	R	1608	3	19,19,19	0.75	0	22,22,22	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	901	-	-	0/6/14/14	0/1/1/1
6	SO4	B	810	-	-	0/0/0/0	0/0/0/0
4	MES	C	902	-	-	0/6/14/14	0/1/1/1
6	SO4	D	811	-	-	0/0/0/0	0/0/0/0
4	MES	E	903	-	-	0/6/14/14	0/1/1/1
6	SO4	F	812	-	-	0/0/0/0	0/0/0/0
4	MES	G	904	-	-	0/6/14/14	0/1/1/1
6	SO4	H	813	-	-	0/0/0/0	0/0/0/0
4	MES	I	905	-	-	0/6/14/14	0/1/1/1
6	SO4	J	814	-	-	0/0/0/0	0/0/0/0
4	MES	K	906	-	-	0/6/14/14	0/1/1/1
6	SO4	L	815	-	-	0/0/0/0	0/0/0/0
8	GER	M	1108	3	-	0/20/20/20	0/0/0/0
8	GER	N	1208	3	-	0/20/20/20	0/0/0/0
8	GER	O	1308	3	-	0/20/20/20	0/0/0/0
8	GER	P	1408	3	-	0/20/20/20	0/0/0/0
8	GER	Q	1508	3	-	0/20/20/20	0/0/0/0
8	GER	R	1608	3	-	0/20/20/20	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	906	MES	C7-C8	-3.74	1.39	1.52
4	A	901	MES	C7-C8	-3.67	1.39	1.52
4	G	904	MES	C7-C8	-3.66	1.39	1.52
4	I	905	MES	C7-C8	-3.63	1.39	1.52
4	E	903	MES	C7-C8	-3.60	1.39	1.52
4	C	902	MES	C7-C8	-3.54	1.40	1.52
4	A	901	MES	C3-C2	-2.62	1.39	1.50
4	K	906	MES	C3-C2	-2.60	1.39	1.50
4	C	902	MES	C3-C2	-2.58	1.39	1.50
4	G	904	MES	C3-C2	-2.58	1.39	1.50
4	E	903	MES	C3-C2	-2.54	1.40	1.50
4	I	905	MES	C3-C2	-2.50	1.40	1.50
4	A	901	MES	C5-C6	-2.45	1.40	1.50
4	I	905	MES	C5-C6	-2.44	1.40	1.50
4	E	903	MES	C5-C6	-2.44	1.40	1.50
4	C	902	MES	C5-C6	-2.42	1.40	1.50
4	K	906	MES	C5-C6	-2.42	1.40	1.50
4	G	904	MES	C5-C6	-2.42	1.40	1.50
4	A	901	MES	C7-N4	-2.26	1.42	1.47
4	G	904	MES	C7-N4	-2.16	1.42	1.47
4	C	902	MES	C7-N4	-2.13	1.42	1.47
4	K	906	MES	C7-N4	-2.12	1.42	1.47
4	E	903	MES	C7-N4	-2.09	1.42	1.47
4	I	905	MES	C7-N4	-2.03	1.42	1.47
4	K	906	MES	O1S-S	10.85	1.79	1.45
4	K	906	MES	O2S-S	10.96	1.79	1.45
4	I	905	MES	O1S-S	10.99	1.79	1.45
4	A	901	MES	O1S-S	11.06	1.79	1.45
4	G	904	MES	O1S-S	11.06	1.79	1.45
4	I	905	MES	O2S-S	11.11	1.79	1.45
4	G	904	MES	O2S-S	11.15	1.79	1.45
4	E	903	MES	O1S-S	11.16	1.79	1.45
4	C	902	MES	O1S-S	11.18	1.80	1.45
4	A	901	MES	O2S-S	11.28	1.80	1.45
4	C	902	MES	O2S-S	11.29	1.80	1.45
4	E	903	MES	O2S-S	11.40	1.80	1.45
4	K	906	MES	O3S-S	12.21	1.78	1.46
4	I	905	MES	O3S-S	12.43	1.78	1.46
4	C	902	MES	O3S-S	12.46	1.78	1.46
4	E	903	MES	O3S-S	12.58	1.78	1.46
4	G	904	MES	O3S-S	12.60	1.78	1.46
4	A	901	MES	O3S-S	12.72	1.79	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	905	MES	O3S-S-O2S	-3.52	103.41	111.61
4	K	906	MES	O3S-S-O2S	-3.42	103.64	111.61
4	G	904	MES	O3S-S-O2S	-3.38	103.74	111.61
4	C	902	MES	O3S-S-O2S	-3.36	103.78	111.61
4	E	903	MES	O3S-S-O2S	-3.28	103.98	111.61
4	A	901	MES	O3S-S-O2S	-2.94	104.76	111.61
4	A	901	MES	O2S-S-O1S	-2.44	104.59	113.48
4	G	904	MES	O2S-S-O1S	-2.30	105.09	113.48
4	K	906	MES	O2S-S-O1S	-2.30	105.11	113.48
4	E	903	MES	O2S-S-O1S	-2.29	105.13	113.48
4	I	905	MES	O2S-S-O1S	-2.29	105.13	113.48
4	K	906	MES	O3S-S-O1S	-2.26	106.36	111.61
4	I	905	MES	O3S-S-O1S	-2.24	106.39	111.61
4	C	902	MES	O2S-S-O1S	-2.23	105.35	113.48
4	A	901	MES	O3S-S-O1S	-2.16	106.57	111.61
4	E	903	MES	O3S-S-O1S	-2.05	106.83	111.61
4	G	904	MES	O3S-S-O1S	-2.01	106.94	111.61
4	A	901	MES	C7-C8-S	4.02	124.94	112.51
4	E	903	MES	C7-C8-S	4.03	124.98	112.51
4	I	905	MES	C7-C8-S	4.03	125.00	112.51
4	G	904	MES	C7-C8-S	4.18	125.45	112.51
4	K	906	MES	C7-C8-S	4.20	125.52	112.51
4	C	902	MES	C7-C8-S	4.21	125.55	112.51
4	A	901	MES	O2S-S-C8	5.77	111.83	106.91
4	E	903	MES	O2S-S-C8	6.06	112.08	106.91
4	G	904	MES	O2S-S-C8	6.25	112.24	106.91
4	C	902	MES	O2S-S-C8	6.43	112.39	106.91
4	I	905	MES	O2S-S-C8	6.76	112.67	106.91
4	G	904	MES	O1S-S-C8	6.82	112.72	106.91
4	K	906	MES	O1S-S-C8	7.01	112.88	106.91
4	E	903	MES	O1S-S-C8	7.07	112.94	106.91
4	C	902	MES	O1S-S-C8	7.08	112.94	106.91
4	K	906	MES	O2S-S-C8	7.18	113.03	106.91
4	I	905	MES	O1S-S-C8	7.37	113.19	106.91
4	A	901	MES	O1S-S-C8	7.45	113.26	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	MES	3	0
4	C	902	MES	1	0
4	E	903	MES	2	0
4	G	904	MES	2	0
4	I	905	MES	2	0
4	K	906	MES	1	0
8	M	1108	GER	1	0
8	N	1208	GER	1	0
8	O	1308	GER	1	0
8	P	1408	GER	1	0
8	Q	1508	GER	1	0
8	R	1608	GER	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	314/377 (83%)	-0.35	4 (1%)	79	71	36, 57, 91, 105	0
1	C	314/377 (83%)	-0.39	5 (1%)	74	66	35, 55, 81, 99	0
1	E	314/377 (83%)	-0.35	3 (0%)	84	77	34, 57, 83, 103	0
1	G	314/377 (83%)	-0.32	6 (1%)	70	59	38, 58, 85, 104	0
1	I	314/377 (83%)	-0.42	5 (1%)	74	66	32, 52, 80, 91	0
1	K	314/377 (83%)	-0.56	1 (0%)	94	92	25, 43, 67, 82	0
2	B	346/377 (91%)	-0.34	8 (2%)	64	52	36, 52, 78, 100	0
2	D	346/377 (91%)	-0.29	8 (2%)	64	52	34, 48, 78, 92	0
2	F	346/377 (91%)	-0.30	6 (1%)	73	63	32, 48, 77, 103	0
2	H	346/377 (91%)	-0.01	12 (3%)	48	35	37, 64, 92, 111	0
2	J	346/377 (91%)	-0.29	9 (2%)	59	47	31, 50, 79, 102	0
2	L	346/377 (91%)	-0.41	3 (0%)	85	79	27, 42, 66, 88	0
3	M	6/11 (54%)	0.15	1 (16%)	2	1	52, 58, 82, 89	0
3	N	6/11 (54%)	0.16	1 (16%)	2	1	56, 61, 79, 85	0
3	O	6/11 (54%)	0.15	1 (16%)	2	1	52, 59, 78, 84	0
3	P	6/11 (54%)	0.38	1 (16%)	2	1	64, 68, 89, 92	0
3	Q	6/11 (54%)	0.06	0	100	100	51, 56, 72, 79	0
3	R	6/11 (54%)	-0.00	0	100	100	51, 57, 71, 76	0
All	All	3996/4590 (87%)	-0.33	74 (1%)	70	59	25, 52, 83, 111	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	363	THR	5.2
2	H	108	SER	5.1
2	B	363	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	J	108	SER	4.0
2	J	363	THR	4.0
2	F	88	SER	3.9
1	C	306	HIS	3.9
1	E	306	HIS	3.8
1	G	305	SER	3.8
1	G	306	HIS	3.6
1	E	91	ILE	3.6
2	D	363	THR	3.5
2	H	361	TRP	3.3
1	G	55	PHE	3.2
2	H	88	SER	3.0
1	C	305	SER	3.0
2	B	86	ASP	2.9
2	F	112	GLY	2.9
1	I	306	HIS	2.9
1	G	326	GLN	2.9
3	M	106	THR	2.9
1	A	304	PRO	2.9
2	D	108	SER	2.9
2	L	363	THR	2.8
2	D	88	SER	2.8
2	J	360	SER	2.8
1	I	305	SER	2.7
2	F	40	TYR	2.7
2	L	113	THR	2.7
2	F	363	THR	2.7
2	D	37	PRO	2.7
2	H	127	THR	2.7
2	H	65	ASP	2.6
3	N	206	THR	2.6
1	A	306	HIS	2.6
1	E	304	PRO	2.6
2	H	362	LYS	2.5
3	O	306	THR	2.5
2	L	108	SER	2.5
1	C	329	ASN	2.5
2	J	110	ASN	2.5
2	F	86	ASP	2.4
1	A	305	SER	2.4
1	I	85	SER	2.4
2	J	85	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	406	THR	2.4
2	H	86	ASP	2.4
2	B	112	GLY	2.3
2	J	112	GLY	2.3
1	I	84	PRO	2.3
2	B	84	THR	2.3
2	H	40	TYR	2.3
1	I	328	ASP	2.3
2	D	361	TRP	2.3
2	H	305	LEU	2.3
2	J	84	THR	2.2
2	J	86	ASP	2.2
1	K	306	HIS	2.2
2	D	86	ASP	2.2
1	C	304	PRO	2.2
2	B	113	THR	2.2
1	G	304	PRO	2.2
2	H	113	THR	2.2
1	G	91	ILE	2.2
2	F	84	THR	2.2
2	H	110	ASN	2.2
2	B	362	LYS	2.1
1	C	55	PHE	2.1
2	B	110	ASN	2.1
2	B	40	TYR	2.1
2	J	111	PRO	2.0
1	A	326	GLN	2.0
2	D	110	ASN	2.0
2	D	113	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
4	MES	A	901	12/12	0.90	0.33	12.12	96,103,106,106	0
4	MES	G	904	12/12	0.89	0.34	8.41	97,101,104,104	0
4	MES	E	903	12/12	0.93	0.26	5.35	84,90,94,94	0
4	MES	C	902	12/12	0.92	0.30	4.93	86,93,95,96	0
4	MES	I	905	12/12	0.91	0.28	3.90	78,84,88,89	0
8	GER	R	1608	20/20	0.93	0.34	3.10	47,50,54,54	0
4	MES	K	906	12/12	0.93	0.25	2.97	65,77,83,84	0
8	GER	M	1108	20/20	0.93	0.28	2.13	48,52,61,61	0
8	GER	Q	1508	20/20	0.94	0.29	1.83	47,50,55,56	0
8	GER	O	1308	20/20	0.93	0.26	1.61	48,51,58,60	0
8	GER	N	1208	20/20	0.93	0.29	1.46	49,53,58,59	0
8	GER	P	1408	20/20	0.89	0.31	1.42	61,66,73,73	0
7	CL	C	801	1/1	0.99	0.15	0.45	53,53,53,53	0
6	SO4	F	812	5/5	0.98	0.14	0.29	67,67,68,69	0
6	SO4	D	811	5/5	0.97	0.15	0.25	66,66,67,67	0
6	SO4	B	810	5/5	0.98	0.14	0.17	67,68,68,69	0
6	SO4	L	815	5/5	0.99	0.16	-0.10	54,54,56,56	0
6	SO4	J	814	5/5	0.99	0.13	-0.55	52,52,54,55	0
7	CL	G	804	1/1	0.99	0.11	-0.98	52,52,52,52	0
6	SO4	H	813	5/5	0.99	0.11	-1.05	68,69,69,70	0
7	CL	K	807	1/1	0.98	0.09	-1.70	44,44,44,44	0
7	CL	H	805	1/1	0.96	0.09	-1.73	60,60,60,60	0
7	CL	D	802	1/1	0.99	0.05	-2.08	45,45,45,45	0
7	CL	J	806	1/1	0.96	0.06	-2.21	58,58,58,58	0
5	ZN	D	378	1/1	0.99	0.05	-2.74	66,66,66,66	0
5	ZN	H	378	1/1	0.96	0.04	-2.78	87,87,87,87	0
5	ZN	L	378	1/1	0.98	0.05	-2.85	58,58,58,58	0
5	ZN	F	378	1/1	0.99	0.05	-3.09	78,78,78,78	0
5	ZN	J	378	1/1	0.97	0.05	-3.18	68,68,68,68	0
5	ZN	B	378	1/1	0.99	0.04	-3.53	77,77,77,77	0
7	CL	F	803	1/1	0.98	0.05	-4.11	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.