Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 03:49 AM EDT

PDB ID	:	6AXG
Title	:	Structure of RasGRP4 in complex with HRas
Authors	:	Kondo, Y.; Iwig, J.S.; Kuriyan, J.
Deposited on	:	2017-09-06
Resolution	:	3.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

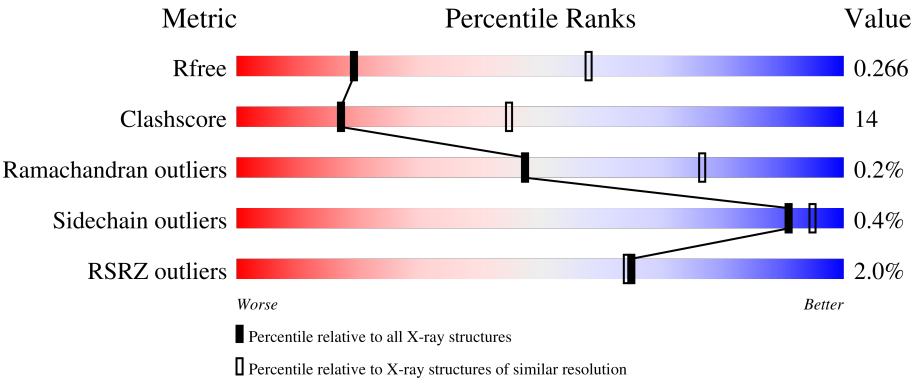
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	418	58% 22% 19%
1	C	418	57% 23% 20%
1	E	418	58% 21% 21%
1	G	418	49% 28% 23%
1	I	418	55% 24% 20%

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Mol	Chain	Length	Quality of chain
1	K	418	2% 53% 27% 19%
2	B	170	% 63% 29% 8%
2	D	170	2% 61% 32% 7%
2	F	170	% 60% 33% 7%
2	H	170	% 57% 34% 8%
2	J	170	2% 63% 29% 8%
2	L	170	3% 59% 32% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23168 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 RAS guanyl-releasing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2659	1678	484	484	13			
1	C	336	Total	C	N	O	S	0	0	0
			2655	1679	484	478	14			
1	E	330	Total	C	N	O	S	0	0	0
			2600	1647	473	467	13			
1	G	320	Total	C	N	O	S	0	0	0
			2552	1621	463	455	13			
1	I	334	Total	C	N	O	S	0	0	0
			2624	1662	477	473	12			
1	K	337	Total	C	N	O	S	0	0	0
			2663	1686	485	478	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	SER	-	expression tag	UNP Q8TDF6
A	44	ASN	-	expression tag	UNP Q8TDF6
A	45	ALA	-	expression tag	UNP Q8TDF6
C	43	SER	-	expression tag	UNP Q8TDF6
C	44	ASN	-	expression tag	UNP Q8TDF6
C	45	ALA	-	expression tag	UNP Q8TDF6
E	43	SER	-	expression tag	UNP Q8TDF6
E	44	ASN	-	expression tag	UNP Q8TDF6
E	45	ALA	-	expression tag	UNP Q8TDF6
G	43	SER	-	expression tag	UNP Q8TDF6
G	44	ASN	-	expression tag	UNP Q8TDF6
G	45	ALA	-	expression tag	UNP Q8TDF6
I	43	SER	-	expression tag	UNP Q8TDF6
I	44	ASN	-	expression tag	UNP Q8TDF6
I	45	ALA	-	expression tag	UNP Q8TDF6
K	43	SER	-	expression tag	UNP Q8TDF6
K	44	ASN	-	expression tag	UNP Q8TDF6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	45	ALA	-	expression tag	UNP Q8TDF6

- Molecule 2 is a protein called GTPase HRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	156	Total	C	N	O	S	0	0	0
			1230	766	214	244	6			
2	D	158	Total	C	N	O	S	0	0	0
			1232	769	207	249	7			
2	F	158	Total	C	N	O	S	0	0	0
			1251	780	215	250	6			
2	H	157	Total	C	N	O	S	0	0	0
			1242	774	213	249	6			
2	J	157	Total	C	N	O	S	0	0	0
			1240	771	216	246	7			
2	L	155	Total	C	N	O	S	0	0	0
			1220	761	212	240	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P01112
B	-2	ALA	-	expression tag	UNP P01112
B	-1	MET	-	expression tag	UNP P01112
B	0	ALA	-	expression tag	UNP P01112
D	-3	GLY	-	expression tag	UNP P01112
D	-2	ALA	-	expression tag	UNP P01112
D	-1	MET	-	expression tag	UNP P01112
D	0	ALA	-	expression tag	UNP P01112
F	-3	GLY	-	expression tag	UNP P01112
F	-2	ALA	-	expression tag	UNP P01112
F	-1	MET	-	expression tag	UNP P01112
F	0	ALA	-	expression tag	UNP P01112
H	-3	GLY	-	expression tag	UNP P01112
H	-2	ALA	-	expression tag	UNP P01112
H	-1	MET	-	expression tag	UNP P01112
H	0	ALA	-	expression tag	UNP P01112
J	-3	GLY	-	expression tag	UNP P01112
J	-2	ALA	-	expression tag	UNP P01112
J	-1	MET	-	expression tag	UNP P01112
J	0	ALA	-	expression tag	UNP P01112
L	-3	GLY	-	expression tag	UNP P01112

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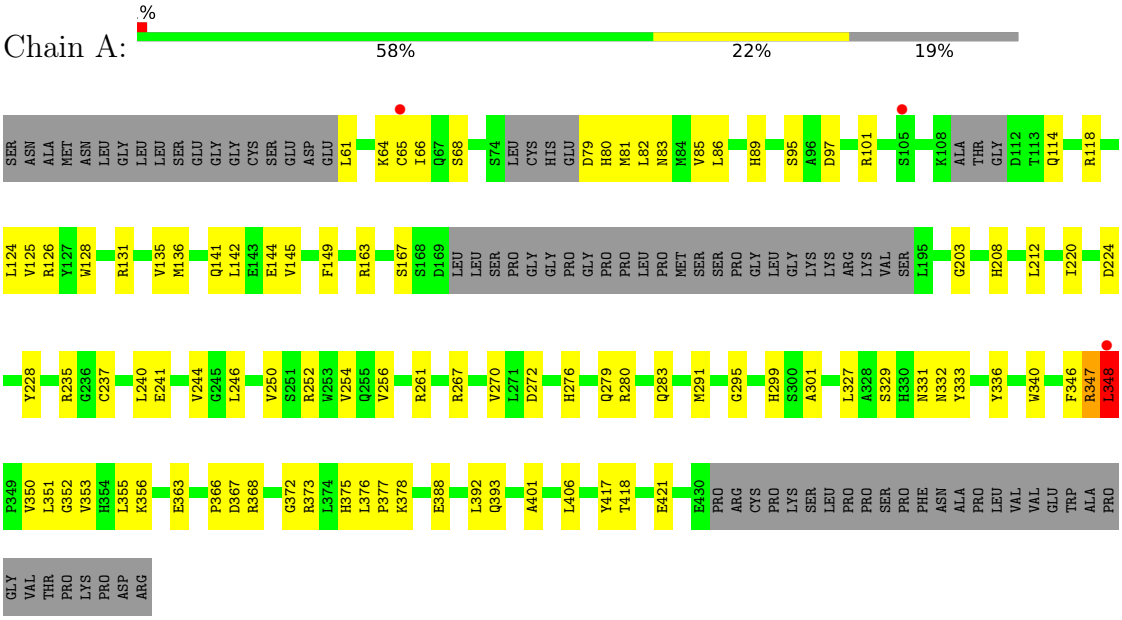
Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	ALA	-	expression tag	UNP P01112
L	-1	MET	-	expression tag	UNP P01112
L	0	ALA	-	expression tag	UNP P01112

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

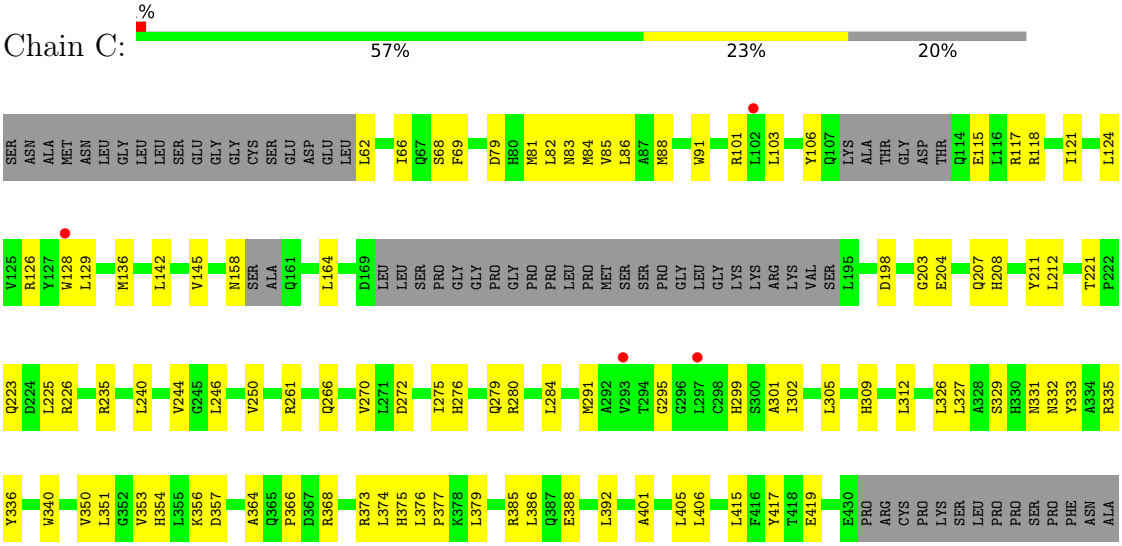
• Molecule 1: RAS guanyl-releasing protein 4

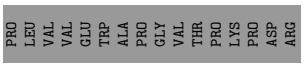
Chain A:



• Molecule 1: RAS guanyl-releasing protein 4

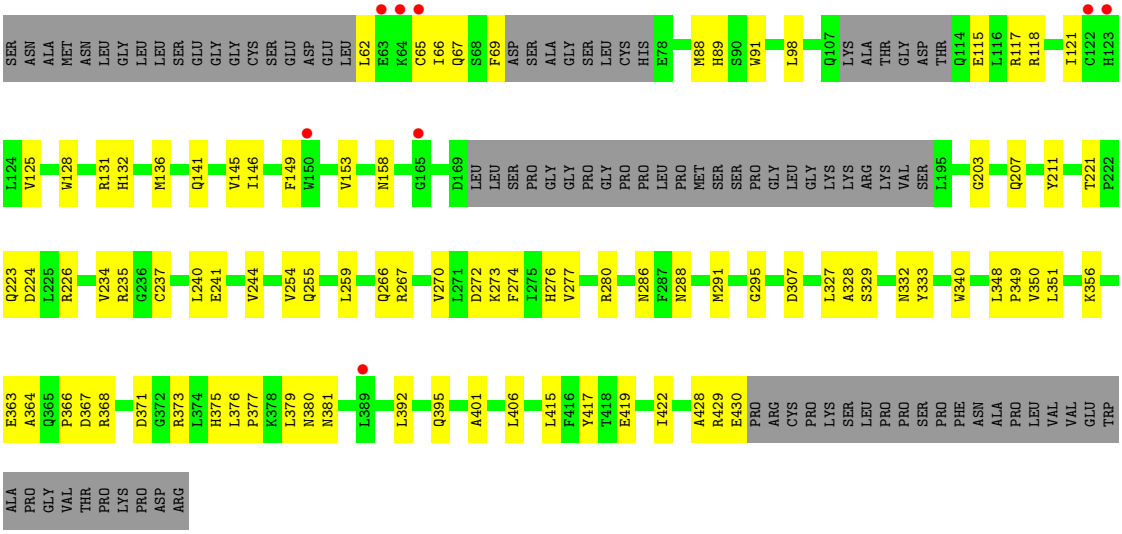
Chain C:





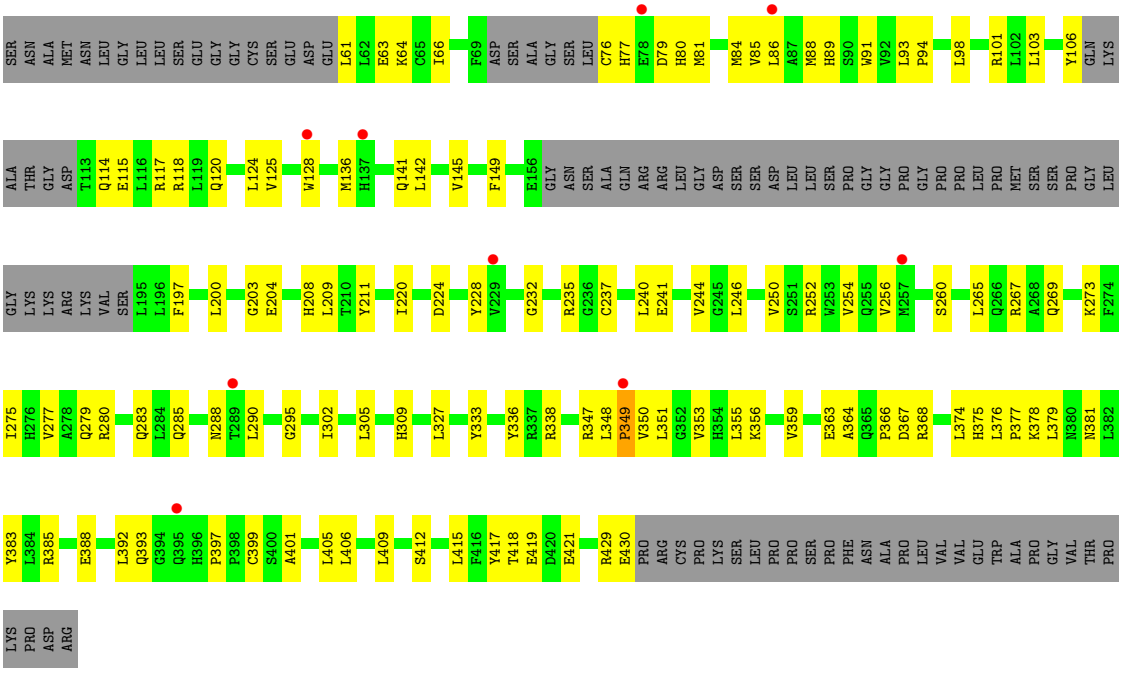
• Molecule 1: RAS guanyl-releasing protein 4

Chain E:



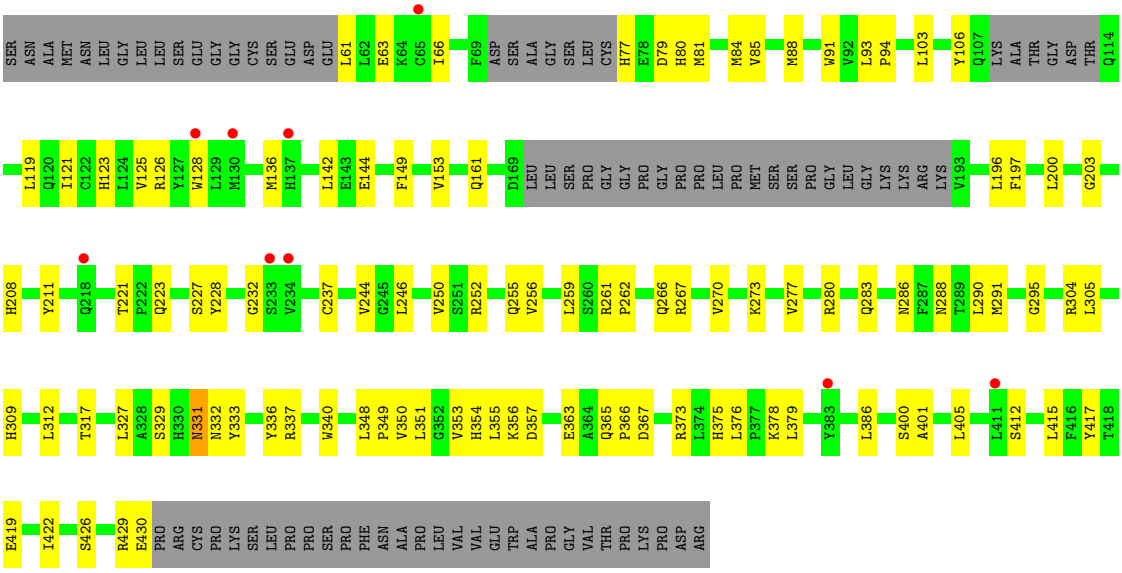
• Molecule 1: RAS guanyl-releasing protein 4

Chain G:



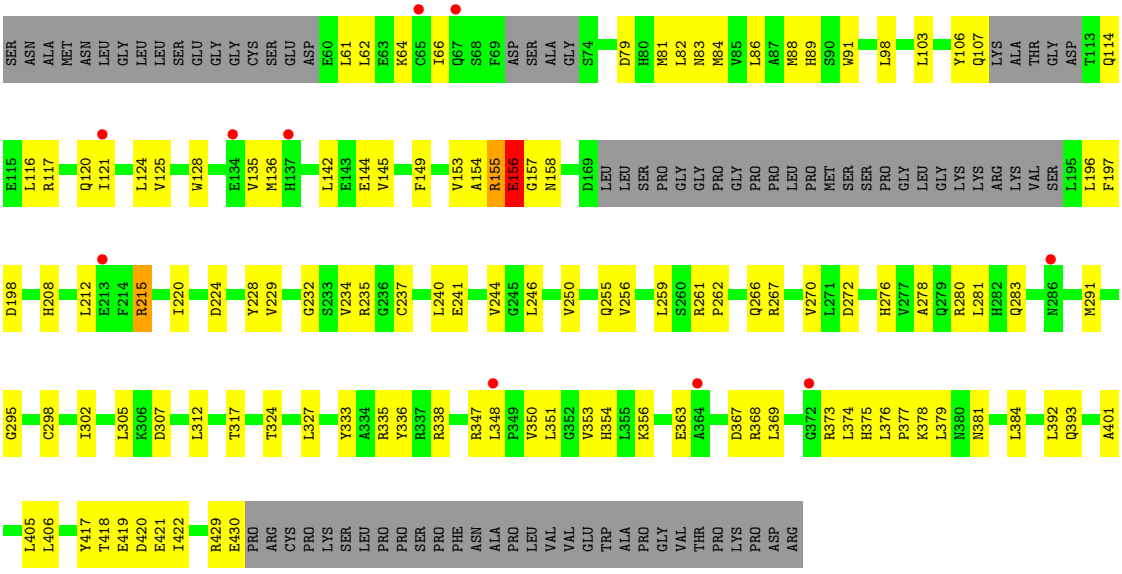
• Molecule 1: RAS guanyl-releasing protein 4

Chain I:



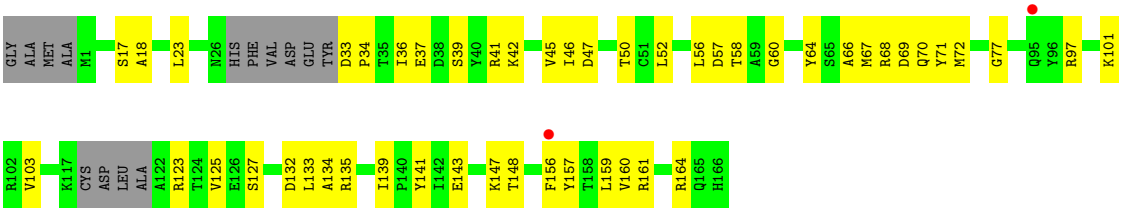
• Molecule 1: RAS guanyl-releasing protein 4

Chain K:



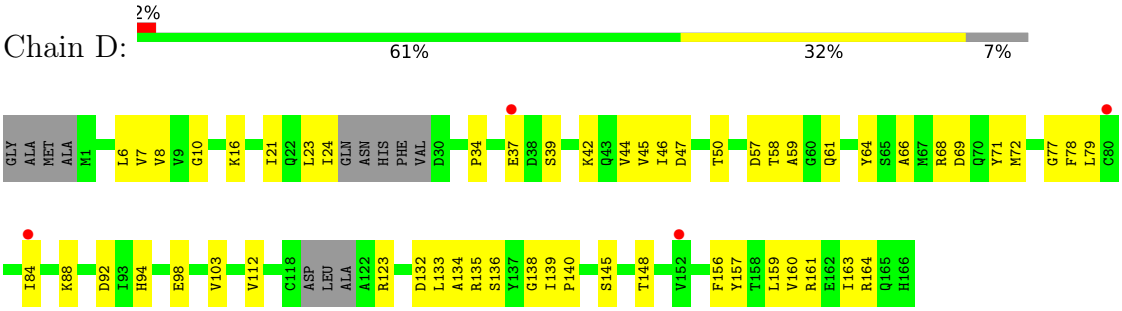
• Molecule 2: GTPase HRas

Chain B:



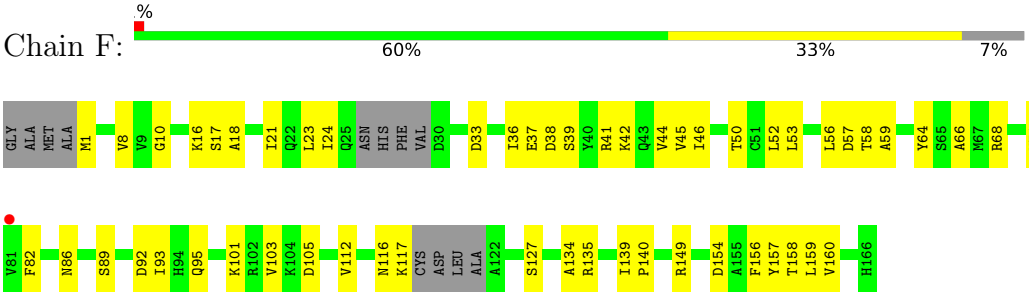
• Molecule 2: GTPase HRas

Chain D:



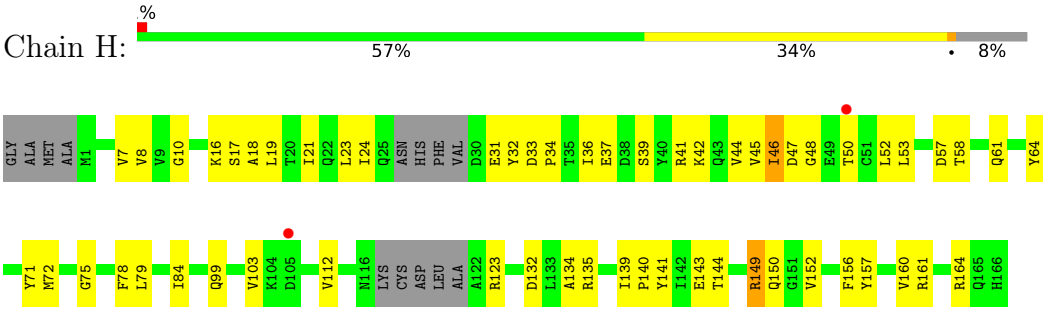
• Molecule 2: GTPase HRas

Chain F:



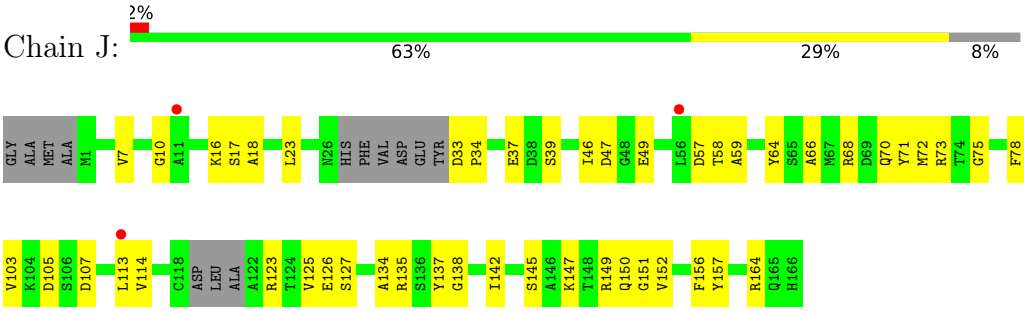
• Molecule 2: GTPase HRas

Chain H:



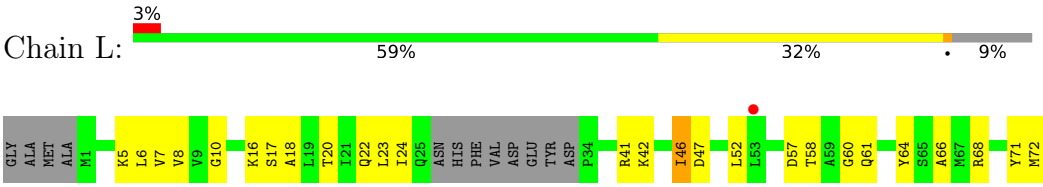
• Molecule 2: GTPase HRas

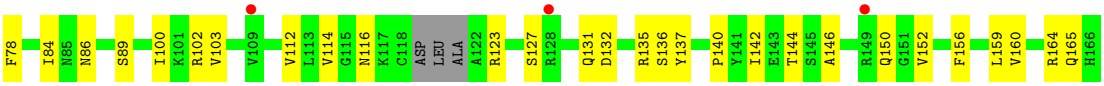
Chain J:



• Molecule 2: GTPase HRas

Chain L:




F78
I84
N85
N86
S89
I100
K101
R102
V103
V109
V112
L113
V114
G115
N116
K117
C118
ASP
LEU
ALA
A122
R123
S127
R128
Q131
D132
R135
S136
Y137
P140
Y141
I142
E143
T144
S145
A146
R149
Q150
G151
V152
F156
L159
V160
R164
Q165
H166

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	114.11Å 114.11Å 680.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.21 – 3.30 49.21 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.21-3.30) 96.3 (49.21-3.30)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.227 , 0.260 0.235 , 0.266	Depositor DCC
R_{free} test set	3814 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	72.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	0.347 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	23168	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.27	0/2716	0.48	0/3687
1	C	0.26	0/2713	0.48	0/3682
1	E	0.26	0/2657	0.46	0/3608
1	G	0.27	0/2610	0.48	0/3545
1	I	0.26	0/2682	0.47	0/3645
1	K	0.26	0/2721	0.47	0/3694
2	B	0.27	0/1244	0.51	0/1675
2	D	0.26	0/1247	0.51	0/1683
2	F	0.26	0/1266	0.48	0/1705
2	H	0.26	0/1257	0.50	0/1694
2	J	0.27	0/1254	0.51	0/1688
2	L	0.26	0/1234	0.55	0/1660
All	All	0.27	0/23601	0.49	0/31966

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	K	0	2
2	H	0	1
2	L	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	LEU	Peptide
1	C	235	ARG	Peptide
2	H	46	ILE	Peptide
1	K	155	ARG	Peptide
1	K	156	GLU	Peptide
2	L	136	SER	Peptide
2	L	46	ILE	Peptide

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	2659	0	2594	81	1
1	C	2655	0	2603	75	0
1	E	2600	0	2544	58	0
1	G	2552	0	2521	85	0
1	I	2624	0	2556	80	1
1	K	2663	0	2616	84	0
2	B	1230	0	1213	41	0
2	D	1232	0	1190	40	0
2	F	1251	0	1226	37	0
2	H	1242	0	1213	46	0
2	J	1240	0	1224	39	0
2	L	1220	0	1209	44	0
All	All	23168	0	22709	636	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 14.

All (636) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:GLY:HA3	2:B:66:ALA:HB1	1.61	0.81
1:C:62:LEU:HB3	1:C:101:ARG:HH12	1.46	0.80
1:G:267:ARG:NH1	1:K:144:GLU:OE2	2.15	0.79
1:E:295:GLY:HA3	2:F:66:ALA:HB1	1.66	0.78
1:I:367:ASP:OD1	1:I:378:LYS:NZ	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:72:MET:HB3	2:J:103:VAL:HG21	1.66	0.78
1:C:295:GLY:HA3	2:D:66:ALA:HB1	1.64	0.77
1:G:348:LEU:HD21	1:G:392:LEU:HD22	1.67	0.77
2:B:72:MET:HB3	2:B:103:VAL:HG21	1.68	0.76
2:B:123:ARG:NH1	2:B:125:VAL:O	2.18	0.76
2:J:49:GLU:OE2	2:L:131:GLN:NE2	2.17	0.76
1:C:299:HIS:ND1	2:D:69:ASP:OD2	2.18	0.76
1:K:228:TYR:HD1	1:K:234:VAL:HG13	1.50	0.76
2:H:72:MET:HB3	2:H:103:VAL:HG21	1.69	0.75
1:G:367:ASP:OD1	1:G:378:LYS:NZ	2.19	0.75
1:A:367:ASP:OD1	1:A:378:LYS:NZ	2.19	0.74
2:D:132:ASP:OD1	2:D:135:ARG:NH2	2.21	0.74
1:E:366:PRO:O	1:E:375:HIS:NE2	2.19	0.74
1:C:419:GLU:OE2	2:D:68:ARG:NH2	2.21	0.74
1:A:224:ASP:HB3	1:A:240:LEU:HD22	1.69	0.74
1:G:204:GLU:O	1:G:208:HIS:ND1	2.21	0.74
1:G:114:GLN:NE2	1:G:115:GLU:OE1	2.21	0.73
1:C:79:ASP:O	1:C:83:ASN:ND2	2.22	0.73
1:A:329:SER:HA	1:A:333:TYR:CE1	2.24	0.73
1:E:291:MET:HE1	1:E:327:LEU:HB3	1.70	0.73
2:L:8:VAL:O	2:L:58:THR:OG1	2.07	0.72
1:K:220:ILE:O	1:K:393:GLN:NE2	2.23	0.71
1:K:244:VAL:HG12	2:L:64:TYR:HE1	1.53	0.71
1:A:83:ASN:OD1	1:A:131:ARG:NH1	2.23	0.71
2:F:135:ARG:NH2	2:H:164:ARG:O	2.24	0.71
1:G:228:TYR:O	1:G:232:GLY:N	2.23	0.70
1:I:244:VAL:HG12	2:J:64:TYR:HE1	1.56	0.70
1:K:267:ARG:NH2	1:K:430:GLU:OE2	2.25	0.70
1:K:234:VAL:HG11	1:K:240:LEU:HD11	1.73	0.70
1:I:331:ASN:ND2	2:J:37:GLU:O	2.24	0.69
2:B:23:LEU:O	2:B:42:LYS:NZ	2.21	0.69
1:A:79:ASP:O	1:A:83:ASN:ND2	2.26	0.69
1:E:348:LEU:HA	1:E:392:LEU:HD22	1.73	0.69
1:I:61:LEU:HG	1:I:373:ARG:HG3	1.75	0.69
1:E:224:ASP:HB3	1:E:240:LEU:HD22	1.75	0.69
1:C:291:MET:HE1	1:C:327:LEU:HB3	1.74	0.69
1:E:234:VAL:HG23	1:E:235:ARG:H	1.57	0.68
1:G:244:VAL:HG12	2:H:64:TYR:HE1	1.58	0.68
1:C:86:LEU:HD13	1:C:128:TRP:HB3	1.74	0.68
2:H:132:ASP:OD1	2:H:135:ARG:NH2	2.27	0.68
2:J:47:ASP:OD2	2:J:164:ARG:NH1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LEU:HD11	1:E:373:ARG:HA	1.74	0.68
1:G:81:MET:HA	1:G:84:MET:HB3	1.75	0.68
1:I:295:GLY:HA3	2:J:66:ALA:HB1	1.75	0.68
1:G:76:CYS:SG	1:G:77:HIS:N	2.67	0.68
1:K:368:ARG:HG2	1:K:374:LEU:HB3	1.76	0.68
2:D:145:SER:OG	2:D:148:THR:OG1	2.10	0.68
1:E:401:ALA:HB1	1:E:406:LEU:HD11	1.74	0.68
1:E:380:ASN:OD1	1:E:381:ASN:N	2.26	0.67
1:I:286:ASN:HA	1:I:349:PRO:HD2	1.76	0.67
1:G:211:TYR:OH	1:G:399:CYS:O	2.11	0.67
1:K:154:ALA:O	1:K:155:ARG:NE	2.27	0.67
1:K:198:ASP:OD2	1:K:261:ARG:NH2	2.27	0.67
1:K:419:GLU:OE2	2:L:68:ARG:NH2	2.28	0.67
1:E:115:GLU:OE2	1:E:158:ASN:ND2	2.23	0.67
2:H:68:ARG:HA	2:H:71:TYR:CE1	2.30	0.67
1:I:329:SER:HA	1:I:333:TYR:CE1	2.29	0.67
1:C:244:VAL:HG12	2:D:64:TYR:HE1	1.59	0.66
1:I:419:GLU:OE2	2:J:68:ARG:NH2	2.24	0.66
2:L:68:ARG:HA	2:L:71:TYR:CE1	2.31	0.66
2:H:10:GLY:O	2:H:16:LYS:NZ	2.24	0.66
1:A:163:ARG:O	1:A:167:SER:CB	2.44	0.66
1:A:244:VAL:HG12	2:B:64:TYR:HE1	1.60	0.66
1:G:429:ARG:HH11	1:K:144:GLU:HG2	1.61	0.66
1:E:415:LEU:HD13	1:E:417:TYR:HD2	1.61	0.65
1:C:204:GLU:O	1:C:208:HIS:ND1	2.29	0.65
1:C:415:LEU:HD13	1:C:417:TYR:HD2	1.60	0.65
1:C:118:ARG:NH2	1:C:158:ASN:O	2.29	0.65
1:I:305:LEU:O	1:I:309:HIS:ND1	2.23	0.65
1:A:299:HIS:ND1	2:B:69:ASP:OD2	2.30	0.65
2:D:47:ASP:OD2	2:D:161:ARG:NE	2.26	0.65
1:G:103:LEU:HD13	1:G:149:PHE:HA	1.77	0.64
1:I:106:TYR:HB2	1:I:121:ILE:HD13	1.78	0.64
2:J:10:GLY:O	2:J:16:LYS:NZ	2.25	0.64
1:G:366:PRO:O	1:G:375:HIS:NE2	2.30	0.64
2:D:23:LEU:O	2:D:42:LYS:NZ	2.27	0.64
1:G:295:GLY:HA3	2:H:66:ALA:HB1	1.79	0.64
2:B:123:ARG:HH22	2:B:127:SER:H	1.45	0.64
1:G:419:GLU:OE2	2:H:68:ARG:NH2	2.31	0.64
1:E:363:GLU:OE1	2:F:17:SER:OG	2.13	0.64
2:H:36:ILE:HG22	2:H:37:GLU:H	1.63	0.64
2:L:84:ILE:HG22	2:L:123:ARG:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:353:VAL:O	1:K:356:LYS:HB3	1.98	0.64
1:A:144:GLU:OE1	1:E:267:ARG:NH1	2.23	0.63
1:I:332:ASN:ND2	2:J:39:SER:OG	2.32	0.63
1:A:346:PHE:HA	1:A:348:LEU:CD2	2.28	0.63
1:I:337:ARG:NH2	1:I:357:ASP:OD1	2.25	0.63
1:G:418:THR:N	1:G:421:GLU:OE1	2.31	0.63
2:J:123:ARG:NH2	2:J:126:GLU:OE1	2.33	0.62
1:K:259:LEU:O	1:K:429:ARG:NE	2.32	0.62
1:I:353:VAL:O	1:I:356:LYS:HB3	1.99	0.62
1:K:401:ALA:HB1	1:K:406:LEU:HD11	1.80	0.62
2:H:24:ILE:HG13	2:H:42:LYS:HE3	1.81	0.62
1:I:203:GLY:HA2	1:I:280:ARG:HG2	1.81	0.62
1:A:332:ASN:ND2	2:B:36:ILE:O	2.33	0.62
2:L:10:GLY:O	2:L:16:LYS:NZ	2.29	0.62
2:J:33:ASP:HB3	2:J:34:PRO:HD3	1.82	0.61
1:I:221:THR:HG22	1:I:223:GLN:H	1.64	0.61
2:D:46:ILE:HG22	2:D:164:ARG:HH22	1.64	0.61
1:G:368:ARG:HG2	1:G:374:LEU:HB3	1.81	0.61
2:J:164:ARG:O	2:L:135:ARG:NH1	2.27	0.61
2:F:33:ASP:O	2:F:39:SER:OG	2.17	0.61
2:J:68:ARG:HA	2:J:71:TYR:CE1	2.35	0.61
1:K:363:GLU:OE1	2:L:17:SER:OG	2.16	0.61
1:K:350:VAL:HG22	1:K:351:LEU:H	1.66	0.61
1:C:221:THR:HG22	1:C:223:GLN:H	1.65	0.60
1:E:371:ASP:HB2	1:E:373:ARG:HG2	1.81	0.60
1:I:80:HIS:O	1:I:84:MET:CB	2.50	0.60
1:I:123:HIS:HA	1:I:126:ARG:HG2	1.83	0.60
1:I:280:ARG:NH1	1:I:283:GLN:OE1	2.32	0.60
1:I:290:LEU:HG	1:I:327:LEU:HD11	1.84	0.60
1:K:272:ASP:O	1:K:276:HIS:ND1	2.31	0.60
1:K:420:ASP:OD1	2:L:102:ARG:NH1	2.30	0.60
1:K:228:TYR:O	1:K:232:GLY:N	2.30	0.60
2:B:47:ASP:HB2	2:B:164:ARG:HH12	1.66	0.60
2:B:68:ARG:HA	2:B:71:TYR:CE1	2.36	0.60
1:C:309:HIS:HA	1:C:312:LEU:HD13	1.84	0.60
2:F:68:ARG:HA	2:F:71:TYR:CE1	2.37	0.60
1:A:61:LEU:O	1:A:65:CYS:N	2.33	0.59
1:K:224:ASP:HB3	1:K:240:LEU:HD22	1.83	0.59
1:K:348:LEU:HB3	1:K:392:LEU:HD22	1.83	0.59
1:E:221:THR:HG22	1:E:223:GLN:H	1.67	0.59
1:C:225:LEU:HD23	1:C:240:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:MET:O	2:B:70:GLN:HG3	2.02	0.59
1:A:331:ASN:HB3	2:B:37:GLU:HB2	1.83	0.59
1:G:220:ILE:O	1:G:393:GLN:NE2	2.31	0.59
2:J:135:ARG:HH11	2:L:165:GLN:HA	1.66	0.59
1:K:367:ASP:OD1	1:K:378:LYS:NZ	2.36	0.59
1:K:103:LEU:O	1:K:106:TYR:HD1	1.86	0.59
1:K:295:GLY:HA3	2:L:66:ALA:HB1	1.84	0.58
2:D:34:PRO:HA	2:D:39:SER:HB3	1.84	0.58
2:J:150:GLN:O	2:J:152:VAL:HG23	2.03	0.58
1:C:82:LEU:HD11	1:C:124:LEU:HD11	1.85	0.58
1:G:349:PRO:O	1:G:350:VAL:HG13	2.03	0.58
1:G:117:ARG:HA	1:G:120:GLN:HB3	1.85	0.58
2:F:36:ILE:HG22	2:F:38:ASP:H	1.68	0.58
2:F:127:SER:HB2	2:H:48:GLY:HA3	1.84	0.58
1:I:88:MET:HE1	1:I:386:LEU:HD22	1.85	0.57
2:H:84:ILE:HD12	2:H:123:ARG:HD3	1.86	0.57
1:C:203:GLY:HA2	1:C:280:ARG:HG2	1.87	0.57
1:C:373:ARG:NH1	1:C:374:LEU:O	2.37	0.57
1:A:135:VAL:HG23	1:A:136:MET:HG3	1.85	0.57
1:C:81:MET:O	1:C:85:VAL:HG23	2.05	0.57
1:C:357:ASP:OD2	1:C:385:ARG:NH2	2.36	0.57
2:J:70:GLN:HG2	2:J:73:ARG:NH2	2.19	0.57
1:K:376:LEU:O	1:K:379:LEU:N	2.38	0.57
1:A:366:PRO:O	1:A:375:HIS:NE2	2.37	0.57
1:K:348:LEU:HD13	1:K:392:LEU:HB3	1.86	0.57
1:G:63:GLU:OE2	1:G:101:ARG:NH1	2.37	0.57
2:D:72:MET:HB3	2:D:103:VAL:HG21	1.86	0.57
1:A:348:LEU:HD23	1:A:348:LEU:H	1.69	0.57
1:E:376:LEU:O	1:E:379:LEU:N	2.38	0.57
1:I:93:LEU:HD12	1:I:94:PRO:HD2	1.87	0.57
2:D:46:ILE:HD11	2:D:157:TYR:CD1	2.40	0.56
1:G:86:LEU:HD13	1:G:128:TRP:HB3	1.86	0.56
2:H:23:LEU:HD13	2:H:152:VAL:HG12	1.87	0.56
1:C:223:GLN:HG3	1:C:226:ARG:HH21	1.70	0.56
1:C:305:LEU:O	1:C:309:HIS:ND1	2.27	0.56
2:F:46:ILE:HD11	2:F:157:TYR:CD1	2.40	0.56
1:I:228:TYR:O	1:I:232:GLY:N	2.33	0.56
1:E:88:MET:SD	1:E:91:TRP:NE1	2.78	0.56
1:K:116:LEU:HD12	1:K:117:ARG:N	2.21	0.56
2:F:72:MET:HB3	2:F:103:VAL:HG21	1.88	0.56
1:A:352:GLY:O	1:A:355:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LEU:O	1:E:429:ARG:NE	2.39	0.56
2:F:82:PHE:HB3	2:F:93:ILE:HD11	1.88	0.56
1:A:346:PHE:HA	1:A:348:LEU:HD21	1.88	0.56
1:K:280:ARG:NH1	1:K:283:GLN:OE1	2.34	0.56
1:C:329:SER:HA	1:C:333:TYR:CE1	2.42	0.55
2:F:8:VAL:HG22	2:F:79:LEU:HD12	1.88	0.55
2:J:46:ILE:HD11	2:J:157:TYR:CD1	2.42	0.55
1:G:197:PHE:HZ	1:G:412:SER:HB3	1.72	0.55
1:G:211:TYR:CD2	1:G:401:ALA:HB3	2.41	0.55
1:G:363:GLU:OE1	2:H:17:SER:OG	2.16	0.55
1:I:88:MET:SD	1:I:91:TRP:NE1	2.80	0.55
1:K:212:LEU:O	1:K:215:ARG:HG3	2.06	0.55
1:A:272:ASP:O	1:A:276:HIS:ND1	2.36	0.55
1:G:415:LEU:HD13	1:G:417:TYR:HD2	1.72	0.55
2:H:34:PRO:HA	2:H:39:SER:HB3	1.89	0.55
2:F:10:GLY:O	2:F:16:LYS:NZ	2.30	0.55
1:C:91:TRP:CH2	1:C:226:ARG:HA	2.41	0.55
1:K:237:CYS:SG	1:K:240:LEU:HD21	2.46	0.55
1:C:136:MET:HG2	1:C:142:LEU:HD22	1.89	0.55
1:I:340:TRP:CZ2	1:I:350:VAL:HG12	2.42	0.55
1:E:136:MET:HE3	1:E:146:ILE:HD11	1.89	0.55
1:G:235:ARG:NH1	1:G:241:GLU:OE2	2.40	0.55
1:G:336:TYR:CE1	1:G:351:LEU:HD13	2.42	0.55
1:A:83:ASN:CG	1:A:131:ARG:HH12	2.09	0.54
1:A:333:TYR:HE2	2:B:67:MET:HE3	1.72	0.54
1:A:348:LEU:HD23	1:A:348:LEU:N	2.21	0.54
1:E:244:VAL:HG12	2:F:64:TYR:HE1	1.70	0.54
1:K:235:ARG:HA	1:K:241:GLU:OE2	2.07	0.54
1:A:299:HIS:HD2	1:A:301:ALA:HB3	1.73	0.54
2:B:97:ARG:HG2	2:B:101:LYS:HE3	1.88	0.54
1:C:366:PRO:O	1:C:375:HIS:NE2	2.41	0.54
2:H:150:GLN:C	2:H:152:VAL:H	2.09	0.54
2:H:41:ARG:HD3	2:H:52:LEU:HD11	1.88	0.54
1:A:353:VAL:O	1:A:356:LYS:HB3	2.08	0.54
2:F:24:ILE:HG13	2:F:42:LYS:HD2	1.89	0.54
1:G:136:MET:HG2	1:G:142:LEU:HD22	1.89	0.54
1:I:366:PRO:O	1:I:375:HIS:NE2	2.40	0.54
2:D:84:ILE:HG22	2:D:123:ARG:HB2	1.88	0.54
1:E:363:GLU:HB3	2:F:18:ALA:HB2	1.89	0.54
1:G:252:ARG:NH1	1:G:415:LEU:O	2.28	0.54
1:K:62:LEU:HD21	1:K:368:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HB3	1:A:392:LEU:HD22	1.89	0.54
1:A:86:LEU:HD22	1:A:128:TRP:CG	2.42	0.54
2:J:70:GLN:HG2	2:J:73:ARG:HH21	1.73	0.54
1:A:388:GLU:O	1:A:392:LEU:HG	2.08	0.53
1:C:62:LEU:HB3	1:C:101:ARG:NH1	2.20	0.53
1:C:198:ASP:OD2	1:C:261:ARG:NH2	2.33	0.53
2:L:7:VAL:HB	2:L:78:PHE:CD1	2.43	0.53
1:G:305:LEU:O	1:G:309:HIS:ND1	2.35	0.53
2:J:123:ARG:NH1	2:J:125:VAL:O	2.41	0.53
1:E:237:CYS:O	1:E:241:GLU:HG3	2.09	0.53
1:G:288:ASN:HB2	1:G:350:VAL:O	2.08	0.53
1:E:272:ASP:O	1:E:276:HIS:ND1	2.35	0.53
2:J:145:SER:O	2:J:150:GLN:HA	2.08	0.53
2:L:24:ILE:HA	2:L:42:LYS:NZ	2.23	0.53
2:B:46:ILE:HD11	2:B:157:TYR:CD2	2.44	0.53
1:I:80:HIS:O	1:I:84:MET:HB2	2.09	0.53
1:G:364:ALA:HA	2:H:21:ILE:HG21	1.90	0.53
2:J:164:ARG:HD3	2:L:131:GLN:HG2	1.90	0.53
2:D:134:ALA:HB1	2:D:139:ILE:O	2.08	0.53
1:I:261:ARG:HD2	1:I:266:GLN:HB3	1.91	0.53
1:I:376:LEU:O	1:I:379:LEU:N	2.42	0.53
2:J:107:ASP:O	2:J:137:TYR:OH	2.26	0.53
1:E:367:ASP:OD1	1:E:368:ARG:N	2.39	0.53
1:G:338:ARG:NH2	2:H:37:GLU:OE2	2.42	0.53
1:I:415:LEU:HD13	1:I:417:TYR:HD2	1.74	0.53
1:K:208:HIS:ND1	1:K:405:LEU:HD22	2.24	0.53
1:A:86:LEU:HD13	1:A:128:TRP:HB2	1.91	0.53
2:B:147:LYS:HD3	2:B:148:THR:HG23	1.91	0.53
2:D:10:GLY:O	2:D:16:LYS:NZ	2.37	0.53
1:G:290:LEU:HG	1:G:327:LEU:HD11	1.89	0.53
2:D:24:ILE:HG13	2:D:42:LYS:HE3	1.90	0.52
2:B:97:ARG:HH22	2:B:133:LEU:HD11	1.74	0.52
1:A:82:LEU:HD21	1:A:124:LEU:HD11	1.92	0.52
1:I:259:LEU:O	1:I:429:ARG:NE	2.43	0.52
1:A:363:GLU:OE1	2:B:17:SER:OG	2.16	0.52
2:L:78:PHE:HD2	2:L:100:ILE:HD13	1.74	0.52
1:E:203:GLY:HA2	1:E:280:ARG:HG2	1.90	0.52
1:G:200:LEU:HD11	1:G:405:LEU:HD21	1.90	0.52
1:G:333:TYR:HE2	2:H:61:GLN:NE2	2.07	0.52
1:A:97:ASP:O	1:A:101:ARG:HG3	2.10	0.52
2:J:46:ILE:HG22	2:J:164:ARG:HH22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:SER:OG	1:C:81:MET:SD	2.56	0.52
1:G:305:LEU:HA	1:G:430:GLU:OE1	2.10	0.52
1:G:376:LEU:HG	1:G:377:PRO:HD3	1.92	0.52
2:H:23:LEU:O	2:H:42:LYS:NZ	2.42	0.52
1:K:61:LEU:HA	1:K:64:LYS:HB2	1.92	0.52
1:A:228:TYR:OH	2:B:60:GLY:HA2	2.10	0.51
1:I:262:PRO:HA	1:I:429:ARG:NH1	2.25	0.51
2:L:127:SER:O	2:L:131:GLN:HG3	2.10	0.51
2:H:46:ILE:HG12	2:H:47:ASP:H	1.73	0.51
1:K:116:LEU:HD12	1:K:117:ARG:H	1.75	0.51
1:I:365:GLN:HB3	1:I:375:HIS:CE1	2.45	0.51
2:L:150:GLN:C	2:L:152:VAL:H	2.13	0.51
1:A:347:ARG:N	1:A:348:LEU:HD23	2.25	0.51
2:D:77:GLY:HA3	2:D:163:ILE:HD11	1.93	0.51
1:G:79:ASP:O	1:G:80:HIS:HB2	2.11	0.51
1:C:142:LEU:HA	1:C:145:VAL:HG22	1.93	0.51
1:E:237:CYS:HB3	1:E:240:LEU:HD21	1.91	0.51
1:G:388:GLU:O	1:G:392:LEU:HG	2.11	0.51
1:G:61:LEU:HA	1:G:64:LYS:HB2	1.91	0.51
1:G:86:LEU:HD13	1:G:128:TRP:CB	2.40	0.51
1:K:155:ARG:NE	1:K:155:ARG:HA	2.24	0.51
2:L:72:MET:HB3	2:L:103:VAL:HG21	1.92	0.51
1:G:200:LEU:HD21	1:G:405:LEU:HD11	1.91	0.51
1:I:200:LEU:HD21	1:I:405:LEU:HD21	1.93	0.51
1:I:291:MET:HB2	1:I:351:LEU:HD21	1.93	0.51
1:K:79:ASP:O	1:K:83:ASN:ND2	2.44	0.51
1:A:329:SER:HA	1:A:333:TYR:CD1	2.46	0.50
1:E:363:GLU:OE1	2:F:18:ALA:N	2.45	0.50
2:H:33:ASP:O	2:H:39:SER:OG	2.20	0.50
1:A:256:VAL:HG11	1:A:417:TYR:HD2	1.74	0.50
1:A:376:LEU:HG	1:A:377:PRO:HD3	1.93	0.50
1:I:80:HIS:O	1:I:84:MET:HB3	2.11	0.50
1:I:88:MET:HA	1:I:91:TRP:HD1	1.76	0.50
1:A:79:ASP:OD1	1:A:80:HIS:N	2.44	0.50
1:A:329:SER:HB3	2:B:70:GLN:HE22	1.76	0.50
2:H:42:LYS:HG2	2:H:44:VAL:HG13	1.93	0.50
1:A:329:SER:HA	1:A:333:TYR:HE1	1.76	0.50
1:C:401:ALA:HB1	1:C:406:LEU:HD11	1.94	0.50
1:I:304:ARG:NH1	1:I:426:SER:OG	2.42	0.50
1:A:348:LEU:CB	1:A:392:LEU:HD22	2.42	0.50
1:A:340:TRP:CH2	1:A:350:VAL:HG12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:348:LEU:HD23	1:I:348:LEU:H	1.76	0.49
2:D:42:LYS:HG2	2:D:44:VAL:HG13	1.94	0.49
2:F:45:VAL:HA	2:F:50:THR:HA	1.94	0.49
1:G:103:LEU:O	1:G:106:TYR:HD1	1.95	0.49
1:I:125:VAL:HA	1:I:128:TRP:CD1	2.47	0.49
1:I:363:GLU:OE1	2:J:18:ALA:HB2	2.13	0.49
1:A:291:MET:HA	1:A:327:LEU:HD13	1.93	0.49
1:A:363:GLU:OE1	2:B:18:ALA:N	2.45	0.49
1:C:326:LEU:HA	1:C:335:ARG:HG2	1.93	0.49
1:K:376:LEU:HA	1:K:379:LEU:HD13	1.95	0.49
1:E:329:SER:HB2	2:F:56:LEU:HD22	1.94	0.49
2:H:45:VAL:HA	2:H:50:THR:HA	1.94	0.49
1:I:106:TYR:HD1	1:I:121:ILE:HG21	1.78	0.49
1:A:299:HIS:CE1	2:B:69:ASP:OD2	2.66	0.49
1:K:228:TYR:OH	2:L:60:GLY:HA2	2.13	0.49
1:K:333:TYR:HE2	2:L:61:GLN:NE2	2.11	0.49
1:I:363:GLU:HG3	2:J:17:SER:OG	2.13	0.49
2:J:123:ARG:HH12	2:J:127:SER:N	2.09	0.49
1:K:81:MET:O	1:K:84:MET:HG3	2.12	0.49
1:C:299:HIS:HD2	1:C:301:ALA:HB3	1.77	0.49
1:G:429:ARG:NH1	1:K:144:GLU:HG2	2.27	0.49
1:A:208:HIS:ND1	1:A:401:ALA:HB1	2.28	0.49
1:C:332:ASN:ND2	2:D:34:PRO:O	2.45	0.49
1:G:208:HIS:CD2	1:G:401:ALA:HB1	2.48	0.49
2:H:31:GLU:O	2:H:32:TYR:HD1	1.95	0.49
1:A:81:MET:O	1:A:85:VAL:HG23	2.12	0.49
1:C:115:GLU:O	1:C:118:ARG:N	2.28	0.49
2:H:8:VAL:HG22	2:H:79:LEU:HD12	1.95	0.49
1:K:61:LEU:HD22	1:K:373:ARG:HD3	1.94	0.48
1:A:329:SER:HB2	2:B:56:LEU:HD22	1.95	0.48
2:B:64:TYR:HD2	2:B:67:MET:SD	2.36	0.48
1:C:272:ASP:O	1:C:276:HIS:ND1	2.46	0.48
1:G:348:LEU:CB	1:G:349:PRO:HA	2.41	0.48
1:C:376:LEU:O	1:C:379:LEU:N	2.45	0.48
2:F:42:LYS:HG2	2:F:44:VAL:HG13	1.94	0.48
1:A:141:GLN:HG3	1:E:428:ALA:O	2.13	0.48
1:C:356:LYS:HD2	2:D:61:GLN:NE2	2.28	0.48
1:I:63:GLU:HA	1:I:66:ILE:HD12	1.95	0.48
2:H:36:ILE:HG22	2:H:37:GLU:N	2.29	0.48
1:E:131:ARG:HG2	1:E:132:HIS:ND1	2.29	0.48
1:G:348:LEU:HB3	1:G:349:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:256:VAL:HG11	1:K:417:TYR:HD2	1.78	0.48
1:K:278:ALA:HA	1:K:281:LEU:HD12	1.95	0.48
2:L:46:ILE:HG22	2:L:47:ASP:H	1.78	0.48
1:C:350:VAL:O	1:C:351:LEU:HG	2.14	0.48
1:E:255:GLN:OE1	1:E:422:ILE:HD13	2.14	0.48
1:K:66:ILE:HD11	1:K:98:LEU:HD22	1.96	0.48
1:G:88:MET:HA	1:G:91:TRP:HD1	1.79	0.48
1:G:256:VAL:O	1:G:260:SER:OG	2.11	0.47
1:I:312:LEU:HD23	1:I:317:THR:HG22	1.95	0.47
1:K:120:GLN:O	1:K:124:LEU:HD13	2.14	0.47
2:B:34:PRO:HA	2:B:39:SER:HB2	1.96	0.47
1:C:329:SER:HA	1:C:333:TYR:CD1	2.49	0.47
1:I:350:VAL:HB	1:I:354:HIS:CD2	2.49	0.47
1:A:261:ARG:HG3	1:A:270:VAL:HG21	1.97	0.47
1:E:125:VAL:HA	1:E:128:TRP:CD1	2.50	0.47
1:I:211:TYR:OH	1:I:400:SER:HA	2.13	0.47
1:I:365:GLN:HB3	1:I:375:HIS:HE1	1.79	0.47
2:J:134:ALA:O	2:J:138:GLY:N	2.45	0.47
1:A:220:ILE:O	1:A:393:GLN:NE2	2.46	0.47
1:G:89:HIS:CD2	1:G:98:LEU:HD12	2.50	0.47
1:A:246:LEU:O	1:A:250:VAL:HG23	2.15	0.47
1:A:368:ARG:NH1	1:A:372:GLY:O	2.37	0.47
1:I:211:TYR:CD2	1:I:401:ALA:HB3	2.49	0.47
1:K:312:LEU:HD23	1:K:317:THR:HG22	1.97	0.47
1:C:356:LYS:HA	2:D:59:ALA:HB3	1.96	0.47
1:I:196:LEU:HD22	1:I:412:SER:OG	2.14	0.47
2:B:57:ASP:OD1	2:B:58:THR:N	2.48	0.47
1:K:302:ILE:HA	1:K:305:LEU:HD13	1.97	0.47
1:E:332:ASN:HB3	2:F:37:GLU:HA	1.95	0.47
1:E:419:GLU:OE2	2:F:68:ARG:NH2	2.48	0.47
1:K:82:LEU:O	1:K:86:LEU:HG	2.15	0.47
1:C:88:MET:HE1	1:C:386:LEU:HD22	1.97	0.47
1:I:197:PHE:CE2	1:I:273:LYS:HD3	2.49	0.47
1:K:142:LEU:HA	1:K:145:VAL:HG22	1.97	0.47
1:C:350:VAL:HG11	1:C:354:HIS:NE2	2.29	0.46
1:E:240:LEU:HD23	1:E:240:LEU:H	1.80	0.46
1:E:288:ASN:HB2	1:E:350:VAL:O	2.14	0.46
1:E:364:ALA:HB2	2:F:21:ILE:HD13	1.97	0.46
2:H:141:TYR:OH	2:H:143:GLU:OE2	2.28	0.46
1:I:136:MET:HG2	1:I:142:LEU:HD22	1.97	0.46
1:I:288:ASN:HB2	1:I:350:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:LEU:HA	1:I:430:GLU:OE1	2.14	0.46
1:E:340:TRP:CZ2	1:E:350:VAL:HG12	2.51	0.46
1:I:252:ARG:NH1	1:I:415:LEU:O	2.45	0.46
1:C:103:LEU:O	1:C:106:TYR:HD1	1.98	0.46
2:D:134:ALA:O	2:D:138:GLY:N	2.44	0.46
1:I:88:MET:HA	1:I:91:TRP:CD1	2.51	0.46
1:I:261:ARG:HG3	1:I:270:VAL:HG21	1.96	0.46
2:L:7:VAL:HG11	2:L:71:TYR:CD2	2.50	0.46
1:A:336:TYR:CE1	1:A:351:LEU:HD13	2.50	0.46
2:D:112:VAL:HG23	2:D:140:PRO:HB2	1.96	0.46
1:G:224:ASP:OD1	1:G:237:CYS:HB2	2.16	0.46
1:K:107:GLN:HB2	1:K:114:GLN:NE2	2.30	0.46
1:I:208:HIS:ND1	1:I:401:ALA:HB1	2.31	0.46
1:C:84:MET:HG3	1:C:85:VAL:N	2.31	0.46
1:C:275:ILE:O	1:C:279:GLN:HG3	2.16	0.46
1:C:364:ALA:HA	2:D:21:ILE:HG21	1.98	0.46
2:D:7:VAL:HB	2:D:78:PHE:CD1	2.51	0.46
1:E:65:CYS:SG	1:E:66:ILE:HG13	2.56	0.46
2:F:57:ASP:OD1	2:F:58:THR:N	2.49	0.46
1:A:89:HIS:NE2	1:A:95:SER:OG	2.33	0.46
2:J:57:ASP:OD1	2:J:58:THR:N	2.48	0.46
1:K:156:GLU:O	1:K:158:ASN:N	2.48	0.46
1:I:149:PHE:O	1:I:153:VAL:HG23	2.16	0.46
2:J:101:LYS:O	2:J:105:ASP:N	2.48	0.46
1:K:298:CYS:SG	1:K:324:THR:OG1	2.68	0.46
2:L:57:ASP:OD1	2:L:58:THR:N	2.49	0.46
2:L:86:ASN:O	2:L:89:SER:OG	2.27	0.46
1:E:356:LYS:HA	2:F:59:ALA:HB3	1.97	0.46
1:E:307:ASP:HB2	1:E:430:GLU:OE2	2.16	0.45
2:H:150:GLN:HA	2:H:152:VAL:HG23	1.98	0.45
1:I:291:MET:HA	1:I:327:LEU:HD13	1.98	0.45
1:C:223:GLN:HG3	1:C:226:ARG:NH2	2.31	0.45
2:D:57:ASP:OD1	2:D:58:THR:N	2.49	0.45
2:F:101:LYS:O	2:F:105:ASP:N	2.48	0.45
1:I:106:TYR:CE2	1:I:153:VAL:HG22	2.51	0.45
1:I:329:SER:HA	1:I:333:TYR:CD1	2.51	0.45
2:J:147:LYS:O	2:J:150:GLN:NE2	2.49	0.45
2:L:41:ARG:HD3	2:L:52:LEU:HD11	1.98	0.45
2:L:114:VAL:HA	2:L:142:ILE:O	2.17	0.45
1:A:61:LEU:HA	1:A:64:LYS:HB3	1.97	0.45
1:A:256:VAL:CG1	1:A:417:TYR:HD2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:VAL:CG1	2:D:16:LYS:HB2	2.46	0.45
1:G:88:MET:HE1	1:G:383:TYR:HA	1.99	0.45
1:G:246:LEU:O	1:G:250:VAL:HG23	2.16	0.45
1:G:355:LEU:O	1:G:359:VAL:HG23	2.17	0.45
2:J:75:GLY:HA3	2:J:78:PHE:HE1	1.81	0.45
1:C:66:ILE:O	1:C:69:PHE:HD1	1.99	0.45
1:E:67:GLN:HA	1:E:69:PHE:CE1	2.51	0.45
1:G:224:ASP:HB3	1:G:240:LEU:HD23	1.97	0.45
1:I:333:TYR:HB3	1:I:336:TYR:HB3	1.98	0.45
1:A:68:SER:OG	1:A:82:LEU:HD23	2.16	0.45
1:A:250:VAL:O	1:A:254:VAL:HG23	2.17	0.45
1:C:81:MET:HA	1:C:84:MET:HG2	1.98	0.45
1:C:353:VAL:O	1:C:356:LYS:HB3	2.16	0.45
1:G:209:LEU:HD23	1:G:409:LEU:HD21	1.98	0.45
2:H:7:VAL:HB	2:H:78:PHE:CD1	2.52	0.45
1:K:135:VAL:HG23	1:K:136:MET:HG3	1.99	0.45
1:K:149:PHE:O	1:K:153:VAL:HG23	2.17	0.45
1:K:240:LEU:HD23	1:K:240:LEU:H	1.80	0.45
1:C:336:TYR:CZ	1:C:351:LEU:HD12	2.52	0.45
1:K:91:TRP:HZ3	1:K:229:VAL:HG11	1.82	0.45
2:L:23:LEU:HD22	2:L:156:PHE:CG	2.52	0.45
1:A:89:HIS:CD2	1:A:95:SER:HG	2.30	0.45
1:C:86:LEU:HD13	1:C:128:TRP:CB	2.42	0.45
1:C:129:LEU:HD11	1:C:136:MET:SD	2.57	0.45
1:C:203:GLY:O	1:C:207:GLN:HG3	2.17	0.45
1:I:106:TYR:CD1	1:I:121:ILE:HG21	2.52	0.45
1:A:61:LEU:HD22	1:A:373:ARG:HB2	1.99	0.45
1:A:142:LEU:HA	1:A:145:VAL:HG22	1.98	0.45
2:D:133:LEU:O	2:D:136:SER:HB3	2.17	0.45
1:G:244:VAL:HG12	2:H:64:TYR:CE1	2.44	0.45
1:G:401:ALA:HB1	1:G:406:LEU:HD11	1.99	0.45
1:K:266:GLN:O	1:K:270:VAL:HG23	2.17	0.45
1:K:376:LEU:HG	1:K:377:PRO:HD3	1.99	0.45
1:A:237:CYS:O	1:A:241:GLU:HG3	2.16	0.44
2:D:8:VAL:HG22	2:D:79:LEU:HD12	1.99	0.44
1:E:288:ASN:HA	1:E:351:LEU:HD23	1.98	0.44
2:H:57:ASP:OD1	2:H:58:THR:N	2.50	0.44
1:K:369:LEU:HD11	1:K:375:HIS:HB3	1.99	0.44
1:A:333:TYR:HB3	1:A:336:TYR:HB3	1.98	0.44
2:B:132:ASP:OD1	2:B:135:ARG:NH2	2.50	0.44
1:C:331:ASN:HB3	2:D:37:GLU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:ASN:OD1	2:F:117:LYS:N	2.50	0.44
1:G:203:GLY:HA2	1:G:280:ARG:HG2	1.97	0.44
1:I:81:MET:O	1:I:85:VAL:HG23	2.16	0.44
1:K:307:ASP:HB2	1:K:430:GLU:OE2	2.16	0.44
2:B:134:ALA:HB1	2:B:139:ILE:O	2.18	0.44
1:C:302:ILE:HA	1:C:305:LEU:HD13	1.99	0.44
2:H:99:GLN:O	2:H:103:VAL:HG13	2.18	0.44
1:I:356:LYS:HA	2:J:59:ALA:HB3	2.00	0.44
1:C:246:LEU:O	1:C:250:VAL:HG23	2.17	0.44
2:F:134:ALA:HB1	2:F:139:ILE:O	2.16	0.44
1:K:121:ILE:O	1:K:125:VAL:HG23	2.18	0.44
2:B:147:LYS:CD	2:B:148:THR:HG23	2.48	0.44
1:E:203:GLY:O	1:E:207:GLN:HG3	2.17	0.44
1:E:244:VAL:HG12	2:F:64:TYR:CE1	2.51	0.44
2:H:157:TYR:O	2:H:161:ARG:HG3	2.17	0.44
1:K:228:TYR:CD1	1:K:234:VAL:HG13	2.41	0.44
1:G:115:GLU:HB3	1:G:118:ARG:HH21	1.83	0.44
1:A:61:LEU:HD12	1:A:64:LYS:HB3	1.99	0.44
1:C:212:LEU:HD12	1:C:406:LEU:HG	1.98	0.44
1:K:335:ARG:O	1:K:338:ARG:HB3	2.18	0.44
1:C:126:ARG:HD2	1:C:164:LEU:CB	2.47	0.44
2:F:112:VAL:HG12	2:F:159:LEU:HD13	1.99	0.44
1:G:250:VAL:O	1:G:254:VAL:HG23	2.18	0.44
1:G:279:GLN:O	1:G:283:GLN:HG3	2.18	0.44
2:L:132:ASP:O	2:L:135:ARG:HG2	2.17	0.44
1:G:93:LEU:HD12	1:G:94:PRO:HD2	1.99	0.43
1:A:291:MET:HE2	1:A:327:LEU:HD22	1.99	0.43
1:C:207:GLN:HE21	1:C:280:ARG:HH21	1.65	0.43
1:C:336:TYR:CE1	1:C:351:LEU:HD12	2.53	0.43
1:E:211:TYR:CD2	1:E:406:LEU:HD21	2.52	0.43
2:H:144:THR:HA	2:H:149:ARG:HD2	2.00	0.43
1:C:280:ARG:NH1	1:C:284:LEU:HG	2.33	0.43
2:D:68:ARG:HA	2:D:71:TYR:CE1	2.53	0.43
1:G:381:ASN:O	1:G:385:ARG:HG2	2.18	0.43
1:I:119:LEU:HG	1:I:123:HIS:HD2	1.84	0.43
1:A:114:GLN:O	1:A:118:ARG:HG3	2.18	0.43
1:C:340:TRP:CH2	1:C:350:VAL:HG22	2.53	0.43
1:I:77:HIS:ND1	1:I:79:ASP:OD2	2.50	0.43
1:I:246:LEU:O	1:I:250:VAL:HG23	2.19	0.43
1:K:246:LEU:O	1:K:250:VAL:HG23	2.18	0.43
2:L:150:GLN:HA	2:L:152:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ILE:HD11	2:B:157:TYR:CG	2.54	0.43
2:B:141:TYR:OH	2:B:143:GLU:OE2	2.30	0.43
1:C:266:GLN:O	1:C:270:VAL:HG23	2.19	0.43
1:I:103:LEU:HD13	1:I:149:PHE:HA	2.00	0.43
1:A:252:ARG:O	1:A:256:VAL:HG13	2.18	0.43
2:D:94:HIS:O	2:D:98:GLU:HG2	2.19	0.43
2:J:23:LEU:HD22	2:J:156:PHE:CG	2.54	0.43
1:K:196:LEU:HD12	1:K:197:PHE:N	2.33	0.43
1:A:212:LEU:HD12	1:A:406:LEU:HG	2.00	0.43
1:C:376:LEU:HG	1:C:377:PRO:HD3	2.01	0.43
2:D:45:VAL:HA	2:D:50:THR:HA	2.00	0.43
2:D:156:PHE:O	2:D:160:VAL:HG23	2.19	0.43
1:I:153:VAL:HG12	1:I:161:GLN:CB	2.49	0.43
1:I:228:TYR:CD2	1:I:355:LEU:HD22	2.54	0.43
1:K:237:CYS:O	1:K:241:GLU:HG3	2.18	0.43
1:K:333:TYR:HB3	1:K:336:TYR:HB3	2.00	0.43
2:L:6:LEU:HD22	2:L:159:LEU:HD23	2.00	0.43
2:L:112:VAL:HG23	2:L:140:PRO:O	2.18	0.43
1:A:346:PHE:HA	1:A:348:LEU:HD23	2.00	0.43
1:E:89:HIS:CD2	1:E:98:LEU:HD12	2.54	0.43
1:G:125:VAL:HA	1:G:128:TRP:CD1	2.54	0.43
1:G:353:VAL:O	1:G:356:LYS:HB3	2.18	0.43
2:J:114:VAL:HA	2:J:142:ILE:O	2.18	0.43
1:E:286:ASN:HA	1:E:349:PRO:HB2	2.01	0.43
1:G:285:GLN:HB3	1:G:347:ARG:HA	2.00	0.43
1:I:415:LEU:HD13	1:I:417:TYR:CD2	2.53	0.43
1:K:291:MET:HA	1:K:327:LEU:HD13	2.01	0.43
2:B:45:VAL:HA	2:B:50:THR:HA	1.99	0.42
1:C:261:ARG:HG3	1:C:270:VAL:HG21	2.00	0.42
1:C:299:HIS:CD2	1:C:301:ALA:H	2.36	0.42
1:K:125:VAL:HA	1:K:128:TRP:CD1	2.54	0.42
1:K:350:VAL:HG21	1:K:354:HIS:NE2	2.34	0.42
2:L:5:LYS:HB2	2:L:76:GLU:HG3	2.00	0.42
1:K:89:HIS:CD2	1:K:98:LEU:HD12	2.53	0.42
2:L:156:PHE:O	2:L:160:VAL:HG23	2.19	0.42
1:G:275:ILE:O	1:G:279:GLN:HG3	2.19	0.42
2:H:112:VAL:HG23	2:H:140:PRO:HB2	2.01	0.42
2:J:7:VAL:HB	2:J:78:PHE:CD1	2.55	0.42
1:C:244:VAL:HG12	2:D:64:TYR:CE1	2.47	0.42
1:C:388:GLU:O	1:C:392:LEU:HG	2.19	0.42
2:D:7:VAL:HG11	2:D:71:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:ASN:O	2:F:89:SER:OG	2.28	0.42
1:G:124:LEU:HD23	1:G:124:LEU:HA	1.74	0.42
1:E:392:LEU:HA	1:E:395:GLN:OE1	2.20	0.42
1:G:63:GLU:OE1	1:G:63:GLU:N	2.53	0.42
1:K:363:GLU:OE1	2:L:18:ALA:N	2.52	0.42
1:A:66:ILE:O	1:A:68:SER:N	2.47	0.42
2:F:41:ARG:HA	2:F:53:LEU:O	2.19	0.42
1:K:235:ARG:HD2	1:K:241:GLU:OE2	2.20	0.42
1:A:235:ARG:HA	1:A:241:GLU:OE2	2.19	0.42
1:A:279:GLN:O	1:A:283:GLN:HG3	2.20	0.42
2:B:33:ASP:O	2:B:36:ILE:HG12	2.20	0.42
1:E:149:PHE:O	1:E:153:VAL:HG23	2.19	0.42
2:F:92:ASP:O	2:F:95:GLN:HG2	2.19	0.42
2:F:112:VAL:HG23	2:F:140:PRO:HB2	2.01	0.42
1:G:115:GLU:O	1:G:118:ARG:HG2	2.20	0.42
1:G:376:LEU:O	1:G:379:LEU:N	2.53	0.42
2:J:123:ARG:HH22	2:J:126:GLU:HA	1.85	0.42
1:K:244:VAL:HG12	2:L:64:TYR:CE1	2.43	0.42
1:K:418:THR:N	1:K:421:GLU:OE1	2.53	0.42
1:A:126:ARG:HH11	1:A:163:ARG:CB	2.32	0.42
1:C:368:ARG:HG2	1:C:374:LEU:HB3	2.01	0.42
2:D:8:VAL:O	2:D:58:THR:OG1	2.35	0.42
1:G:63:GLU:HA	1:G:66:ILE:HB	2.01	0.42
1:K:88:MET:HA	1:K:91:TRP:CD1	2.55	0.42
1:K:333:TYR:HE2	2:L:61:GLN:HE22	1.66	0.42
2:L:46:ILE:HG22	2:L:164:ARG:HH22	1.85	0.42
2:B:47:ASP:OD2	2:B:161:ARG:NE	2.38	0.42
2:B:77:GLY:C	2:B:159:LEU:HD21	2.40	0.42
2:D:8:VAL:HG12	2:D:16:LYS:HB2	2.02	0.42
2:F:156:PHE:O	2:F:160:VAL:HG23	2.20	0.42
1:G:280:ARG:NH1	1:G:283:GLN:OE1	2.46	0.42
1:G:302:ILE:HA	1:G:305:LEU:HD13	2.01	0.42
2:L:22:GLN:NE2	2:L:146:ALA:O	2.45	0.42
2:J:80:CYS:O	2:J:113:LEU:HD12	2.19	0.41
1:E:224:ASP:HB3	1:E:240:LEU:CD2	2.48	0.41
2:H:41:ARG:HA	2:H:53:LEU:O	2.20	0.41
1:K:381:ASN:O	1:K:384:LEU:HG	2.20	0.41
1:A:125:VAL:HG21	1:A:149:PHE:CE2	2.55	0.41
2:H:19:LEU:HD12	2:H:152:VAL:HG22	2.02	0.41
2:H:75:GLY:HA3	2:H:78:PHE:HE1	1.86	0.41
1:I:256:VAL:HG11	1:I:417:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:418:THR:HG22	1:K:419:GLU:H	1.85	0.41
1:E:328:ALA:O	1:E:333:TYR:HA	2.20	0.41
2:H:24:ILE:HA	2:H:42:LYS:NZ	2.34	0.41
2:H:156:PHE:O	2:H:160:VAL:HG23	2.19	0.41
1:I:125:VAL:HA	1:I:128:TRP:HD1	1.85	0.41
1:I:255:GLN:OE1	1:I:422:ILE:HD13	2.20	0.41
1:K:255:GLN:OE1	1:K:422:ILE:HD13	2.20	0.41
2:L:116:ASN:HA	2:L:144:THR:O	2.20	0.41
2:B:17:SER:HB3	2:B:57:ASP:OD2	2.20	0.41
1:E:254:VAL:HG22	1:E:274:PHE:CE1	2.55	0.41
2:F:23:LEU:HD22	2:F:156:PHE:CG	2.55	0.41
1:I:261:ARG:HB2	1:I:267:ARG:HG2	2.03	0.41
1:I:333:TYR:CE2	1:I:353:VAL:HG11	2.55	0.41
2:L:41:ARG:CD	2:L:52:LEU:HD21	2.51	0.41
1:C:208:HIS:CD2	1:C:405:LEU:HD22	2.56	0.41
1:C:211:TYR:HD2	1:C:406:LEU:HD21	1.84	0.41
2:D:6:LEU:HD22	2:D:159:LEU:HD23	2.03	0.41
1:G:363:GLU:OE1	2:H:18:ALA:N	2.53	0.41
1:K:262:PRO:O	1:K:267:ARG:NH1	2.53	0.41
1:K:375:HIS:CE1	1:K:378:LYS:HB2	2.55	0.41
2:L:23:LEU:HD22	2:L:156:PHE:CD2	2.56	0.41
1:A:82:LEU:HD21	1:A:124:LEU:CD1	2.51	0.41
1:G:348:LEU:HD23	1:G:348:LEU:HA	1.81	0.41
1:G:351:LEU:HD23	2:H:67:MET:HE2	2.03	0.41
1:G:81:MET:O	1:G:85:VAL:HG23	2.20	0.41
1:G:273:LYS:O	1:G:277:VAL:HG23	2.21	0.41
2:H:134:ALA:HB1	2:H:139:ILE:O	2.21	0.41
1:A:244:VAL:HG12	2:B:64:TYR:CE1	2.49	0.41
2:B:46:ILE:HD13	2:B:46:ILE:HA	1.78	0.41
1:G:211:TYR:HE1	1:G:397:PRO:HB2	1.86	0.41
2:J:23:LEU:HD13	2:J:152:VAL:HG12	2.02	0.41
2:J:123:ARG:NH2	2:J:126:GLU:HA	2.36	0.41
1:A:418:THR:N	1:A:421:GLU:OE1	2.30	0.41
1:C:115:GLU:O	1:C:117:ARG:N	2.54	0.41
2:D:88:LYS:HE3	2:D:92:ASP:OD1	2.21	0.41
1:E:117:ARG:O	1:E:121:ILE:HG12	2.21	0.41
1:G:141:GLN:O	1:G:145:VAL:HG22	2.20	0.41
1:I:266:GLN:O	1:I:270:VAL:HG23	2.21	0.41
1:I:273:LYS:O	1:I:277:VAL:HG23	2.21	0.41
1:A:333:TYR:CE2	2:B:67:MET:HE3	2.54	0.40
1:C:117:ARG:O	1:C:121:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:GLN:O	1:E:270:VAL:HG23	2.21	0.40
2:B:41:ARG:HD3	2:B:52:LEU:HD11	2.02	0.40
1:E:141:GLN:O	1:E:145:VAL:HG22	2.22	0.40
1:A:299:HIS:CD2	1:A:301:ALA:H	2.38	0.40
1:E:376:LEU:HG	1:E:377:PRO:HD3	2.02	0.40
1:I:227:SER:HB2	1:I:237:CYS:SG	2.61	0.40
2:L:8:VAL:HG21	2:L:20:THR:OG1	2.20	0.40
1:C:340:TRP:CH2	1:C:350:VAL:HG13	2.57	0.40
2:F:1:MET:SD	2:F:52:LEU:HB2	2.61	0.40
2:H:46:ILE:HG23	2:H:164:ARG:NH2	2.36	0.40
1:A:203:GLY:HA2	1:A:280:ARG:HG2	2.04	0.40
2:B:156:PHE:O	2:B:160:VAL:HG23	2.22	0.40
1:E:273:LYS:O	1:E:277:VAL:HG23	2.21	0.40
2:F:154:ASP:O	2:F:158:THR:OG1	2.29	0.40
1:G:265:LEU:O	1:G:269:GLN:HG3	2.21	0.40
2:L:8:VAL:CG1	2:L:16:LYS:HB2	2.52	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)
1:A:267:ARG:NH1	1:I:144:GLU:OE2[1_565]	2.07	0.13

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	330/418 (79%)	319 (97%)	11 (3%)	0	100	100
1	C	328/418 (78%)	309 (94%)	19 (6%)	0	100	100
1	E	322/418 (77%)	308 (96%)	14 (4%)	0	100	100
1	G	312/418 (75%)	297 (95%)	14 (4%)	1 (0%)	41	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	326/418 (78%)	308 (94%)	18 (6%)	0	100 100
1	K	329/418 (79%)	304 (92%)	23 (7%)	2 (1%)	25 57
2	B	150/170 (88%)	145 (97%)	5 (3%)	0	100 100
2	D	152/170 (89%)	147 (97%)	5 (3%)	0	100 100
2	F	152/170 (89%)	145 (95%)	7 (5%)	0	100 100
2	H	151/170 (89%)	140 (93%)	11 (7%)	0	100 100
2	J	151/170 (89%)	141 (93%)	9 (6%)	1 (1%)	22 54
2	L	149/170 (88%)	140 (94%)	8 (5%)	1 (1%)	22 54
All	All	2852/3528 (81%)	2703 (95%)	144 (5%)	5 (0%)	47 77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	151	GLY
1	G	349	PRO
1	K	156	GLU
1	K	157	GLY
2	L	137	TYR

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	283/362 (78%)	281 (99%)	2 (1%)	84 90
1	C	284/362 (78%)	284 (100%)	0	100 100
1	E	276/362 (76%)	274 (99%)	2 (1%)	84 90
1	G	276/362 (76%)	276 (100%)	0	100 100
1	I	278/362 (77%)	277 (100%)	1 (0%)	91 95
1	K	285/362 (79%)	283 (99%)	2 (1%)	84 90
2	B	133/145 (92%)	133 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	132/145 (91%)	132 (100%)	0	100 100
2	F	135/145 (93%)	134 (99%)	1 (1%)	84 90
2	H	134/145 (92%)	133 (99%)	1 (1%)	84 90
2	J	135/145 (93%)	134 (99%)	1 (1%)	84 90
2	L	132/145 (91%)	132 (100%)	0	100 100
All	All	2483/3042 (82%)	2473 (100%)	10 (0%)	91 95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	ARG
1	A	348	LEU
1	E	118	ARG
1	E	226	ARG
2	F	149	ARG
2	H	149	ARG
1	I	331	ASN
2	J	149	ARG
1	K	215	ARG
1	K	347	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	207	GLN
1	E	396	HIS
2	H	61	GLN
1	I	332	ASN
1	K	114	GLN
2	L	61	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	338/418 (80%)	0.13	3 (0%)	84	84	40, 77, 124, 195	0
1	C	336/418 (80%)	0.16	4 (1%)	79	78	27, 84, 159, 225	0
1	E	330/418 (78%)	0.26	8 (2%)	59	56	46, 92, 147, 226	0
1	G	320/418 (76%)	0.33	9 (2%)	53	51	42, 94, 169, 216	0
1	I	334/418 (79%)	0.22	9 (2%)	54	52	40, 85, 147, 183	0
1	K	337/418 (80%)	0.21	10 (2%)	50	49	45, 81, 146, 212	0
2	B	156/170 (91%)	0.21	2 (1%)	77	77	32, 75, 115, 161	0
2	D	158/170 (92%)	0.21	4 (2%)	57	54	40, 76, 121, 174	0
2	F	158/170 (92%)	0.25	1 (0%)	89	90	61, 89, 134, 181	0
2	H	157/170 (92%)	0.30	2 (1%)	77	77	48, 86, 142, 195	0
2	J	157/170 (92%)	0.34	3 (1%)	66	65	55, 86, 145, 227	0
2	L	155/170 (91%)	0.40	5 (3%)	47	46	57, 84, 124, 169	0
All	All	2936/3528 (83%)	0.24	60 (2%)	65	64	27, 84, 145, 227	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	64	LYS	5.7
1	I	65	CYS	4.2
1	G	128	TRP	4.0
1	G	289	THR	3.9
1	E	63	GLU	3.4
1	G	395	GLN	3.3
1	K	65	CYS	3.2
1	I	128	TRP	3.2
1	C	128	TRP	3.2
2	J	11	ALA	3.1
1	I	233	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	67	GLN	3.0
1	G	349	PRO	2.9
1	K	348	LEU	2.9
2	H	105	ASP	2.9
1	G	137	HIS	2.8
1	E	122	CYS	2.6
1	I	383	TYR	2.6
1	K	121	ILE	2.6
1	I	137	HIS	2.6
1	C	297	LEU	2.6
2	H	50	THR	2.6
2	L	53	LEU	2.5
1	K	137	HIS	2.5
2	B	156	PHE	2.5
2	L	109	VAL	2.5
1	A	348	LEU	2.5
1	I	234	VAL	2.5
1	I	130	MET	2.5
2	J	56	LEU	2.5
1	I	218	GLN	2.5
1	G	257	MET	2.4
1	E	123	HIS	2.4
2	F	81	VAL	2.4
1	C	293	VAL	2.4
2	L	128	ARG	2.4
1	E	65	CYS	2.4
2	J	113	LEU	2.3
1	G	78	GLU	2.3
1	G	86	LEU	2.2
2	L	149	ARG	2.2
2	D	37	GLU	2.2
1	K	134	GLU	2.2
1	K	364	ALA	2.2
1	E	389	LEU	2.2
1	A	105	SER	2.2
1	K	213	GLU	2.2
1	I	411	LEU	2.2
2	B	95	GLN	2.1
1	K	372	GLY	2.1
1	C	102	LEU	2.1
2	L	75	GLY	2.1
1	E	150	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	165	GLY	2.1
1	A	65	CYS	2.0
1	G	229	VAL	2.0
2	D	84	ILE	2.0
2	D	152	VAL	2.0
1	K	286	ASN	2.0
2	D	80	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.