Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2024 – 03:00 pm BST

PDB ID	:	8POO
Title	:	Low resolution structure of inactive conformation of the Ktr cation channel in presence of ATP and c-di-AMP
Authors	:	Cereija, T.B.; Teixeira-Duarte, C.M.; Morais-Cabral, J.H.
Deposited on	:	2023-07-05
Resolution	:	5.77 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:

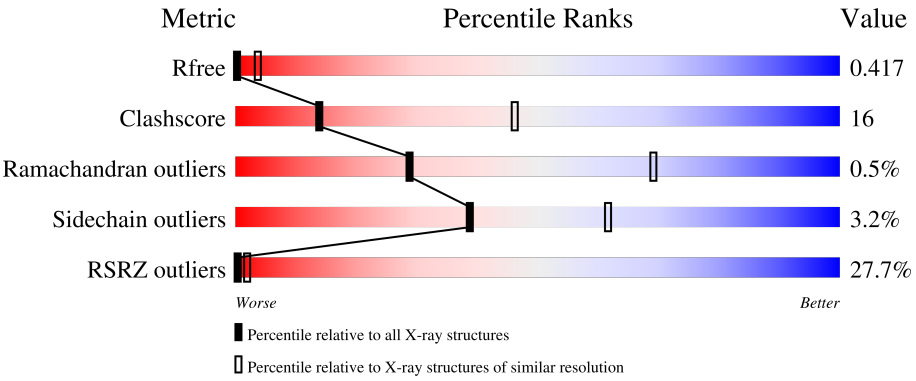
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 5.77 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	1008 (7.70-3.86)
Clashscore	141614	1034 (7.66-3.90)
Ramachandran outliers	138981	1003 (7.70-3.86)
Sidechain outliers	138945	1005 (7.70-3.82)
RSRZ outliers	127900	1005 (7.78-3.78)

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	445	15% 54% 34% · 9%
1	B	445	14% 55% 34% · 9%
1	I	445	17% 60% 29% · 9%
1	J	445	14% 54% 34% · 9%
2	C	288	35% 62% 31% · 7%

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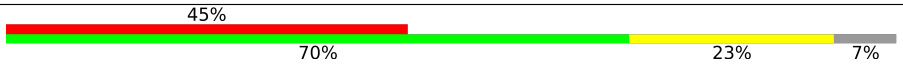
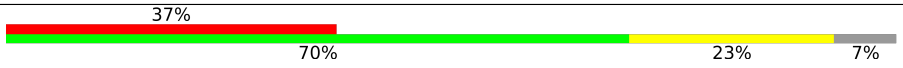
Mol	Chain	Length	Quality of chain
2	D	288	
2	E	288	
2	G	288	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20736 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 Ktr system potassium uptake protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			
1	J	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			
1	A	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			
1	B	406	Total	C	N	O	S	0	0	0
			3088	2064	474	536	14			

- Molecule 2 is a protein called Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
2	D	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
2	E	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			
2	G	268	Total	C	N	O	S	0	0	0
			2096	1336	362	394	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	22	VAL	CYS	engineered mutation	UNP O32080
C	145	LEU	-	linker	UNP O32080
C	146	GLU	-	linker	UNP O32080
C	147	GLY	-	linker	UNP O32080
C	148	SER	-	linker	UNP O32080
C	164	VAL	CYS	engineered mutation	UNP O32080
C	283	LEU	-	expression tag	UNP O32080
C	284	GLU	-	expression tag	UNP O32080

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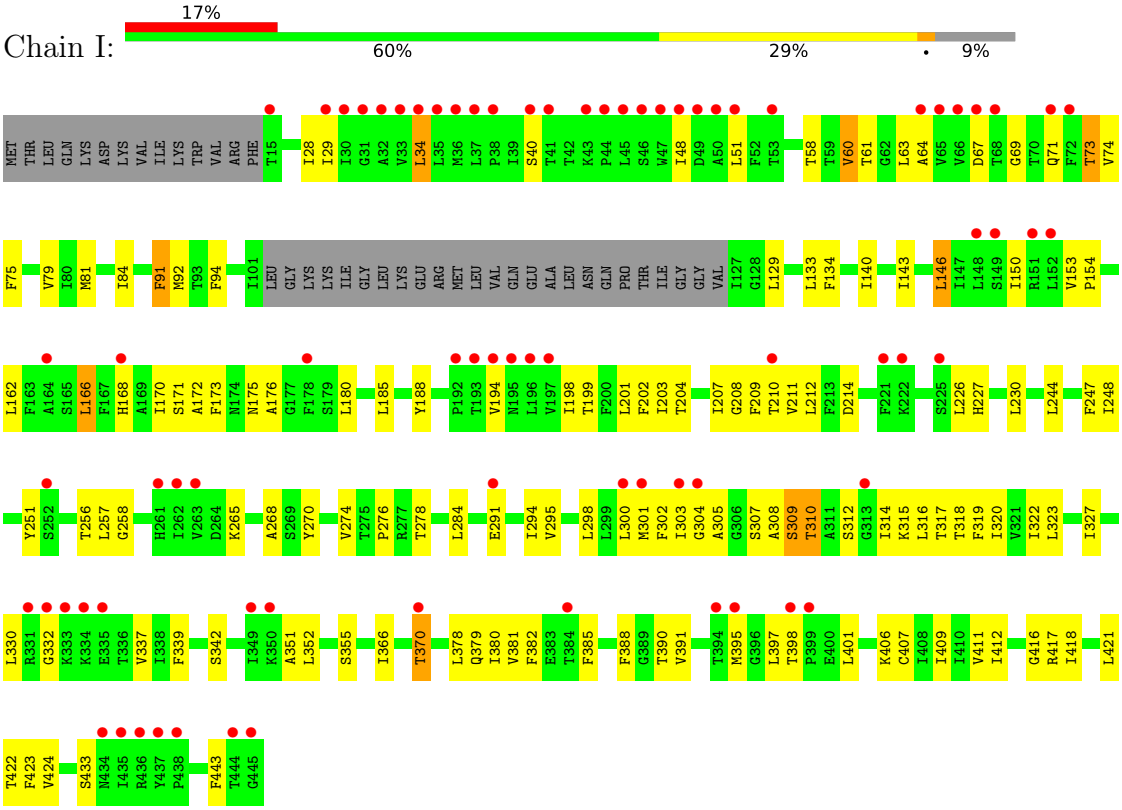
Chain	Residue	Modelled	Actual	Comment	Reference
C	285	LEU	-	expression tag	UNP O32080
C	286	VAL	-	expression tag	UNP O32080
C	287	PRO	-	expression tag	UNP O32080
C	288	ARG	-	expression tag	UNP O32080
D	22	VAL	CYS	engineered mutation	UNP O32080
D	145	LEU	-	linker	UNP O32080
D	146	GLU	-	linker	UNP O32080
D	147	GLY	-	linker	UNP O32080
D	148	SER	-	linker	UNP O32080
D	164	VAL	CYS	engineered mutation	UNP O32080
D	283	LEU	-	expression tag	UNP O32080
D	284	GLU	-	expression tag	UNP O32080
D	285	LEU	-	expression tag	UNP O32080
D	286	VAL	-	expression tag	UNP O32080
D	287	PRO	-	expression tag	UNP O32080
D	288	ARG	-	expression tag	UNP O32080
E	22	VAL	CYS	engineered mutation	UNP O32080
E	145	LEU	-	linker	UNP O32080
E	146	GLU	-	linker	UNP O32080
E	147	GLY	-	linker	UNP O32080
E	148	SER	-	linker	UNP O32080
E	164	VAL	CYS	engineered mutation	UNP O32080
E	283	LEU	-	expression tag	UNP O32080
E	284	GLU	-	expression tag	UNP O32080
E	285	LEU	-	expression tag	UNP O32080
E	286	VAL	-	expression tag	UNP O32080
E	287	PRO	-	expression tag	UNP O32080
E	288	ARG	-	expression tag	UNP O32080
G	22	VAL	CYS	engineered mutation	UNP O32080
G	145	LEU	-	linker	UNP O32080
G	146	GLU	-	linker	UNP O32080
G	147	GLY	-	linker	UNP O32080
G	148	SER	-	linker	UNP O32080
G	164	VAL	CYS	engineered mutation	UNP O32080
G	283	LEU	-	expression tag	UNP O32080
G	284	GLU	-	expression tag	UNP O32080
G	285	LEU	-	expression tag	UNP O32080
G	286	VAL	-	expression tag	UNP O32080
G	287	PRO	-	expression tag	UNP O32080
G	288	ARG	-	expression tag	UNP O32080

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.

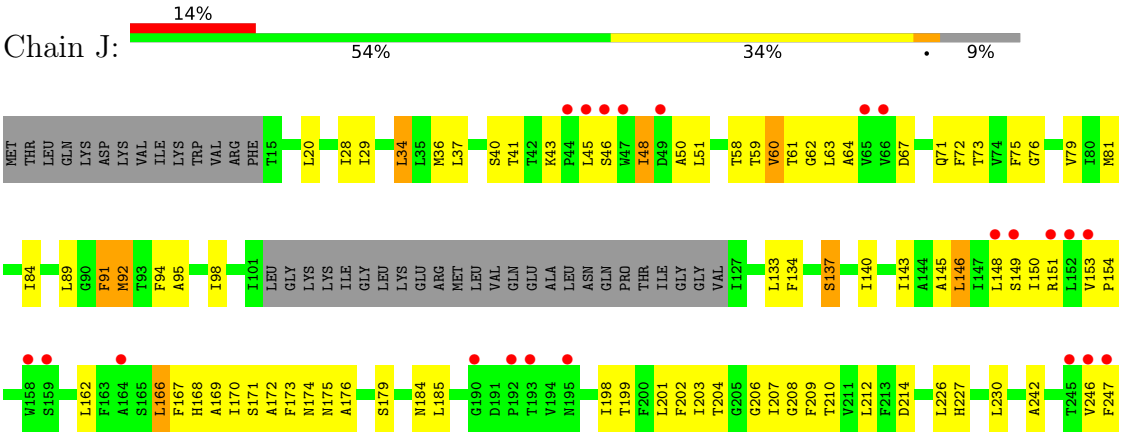
• Molecule 1: Ktr system potassium uptake protein B

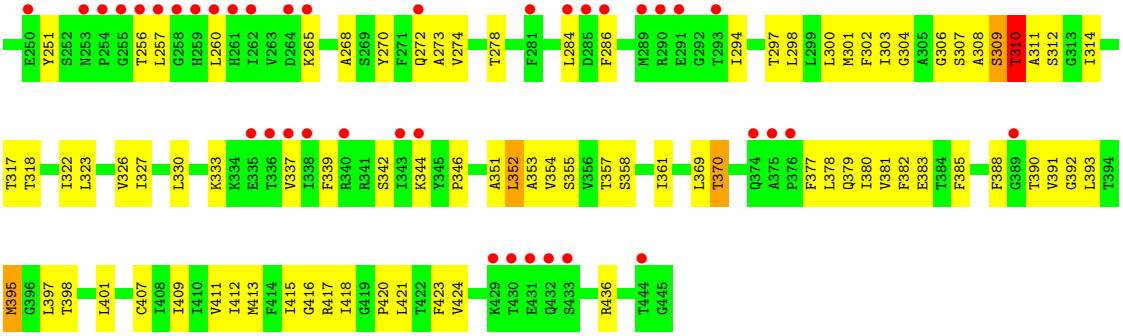
Chain I:



• Molecule 1: Ktr system potassium uptake protein B

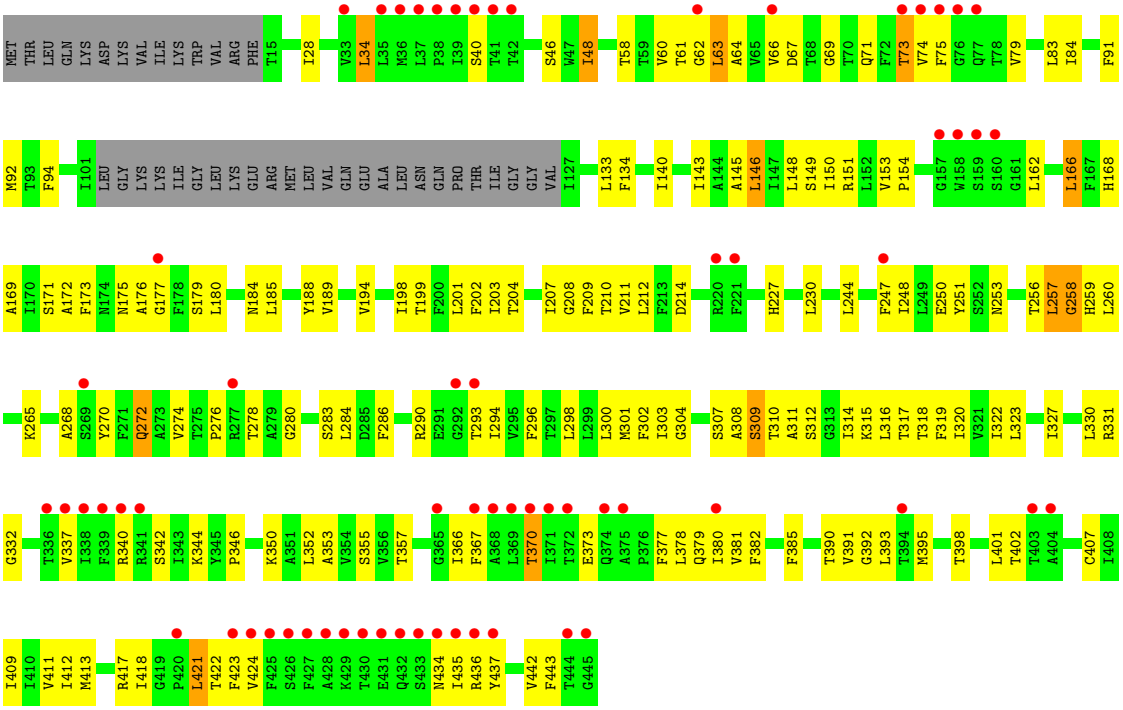
Chain J:





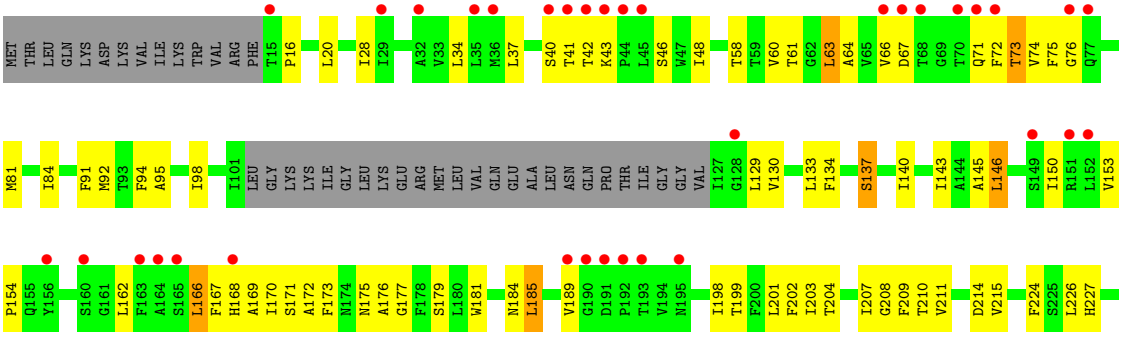
• Molecule 1: Ktr system potassium uptake protein B

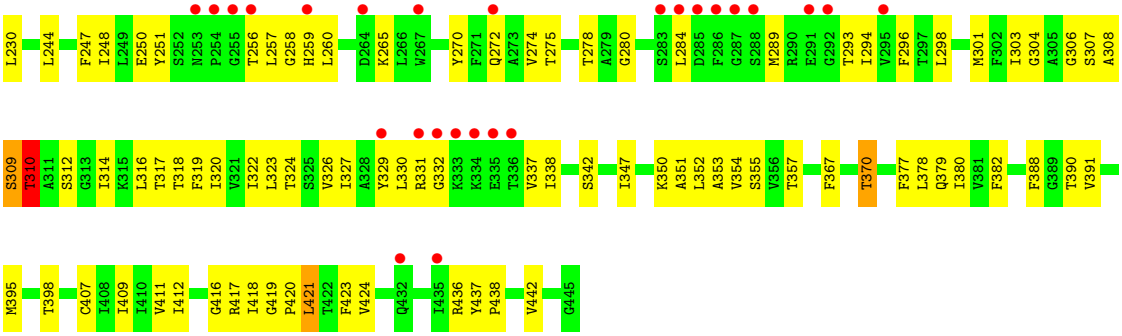
Chain A:



• Molecule 1: Ktr system potassium uptake protein B

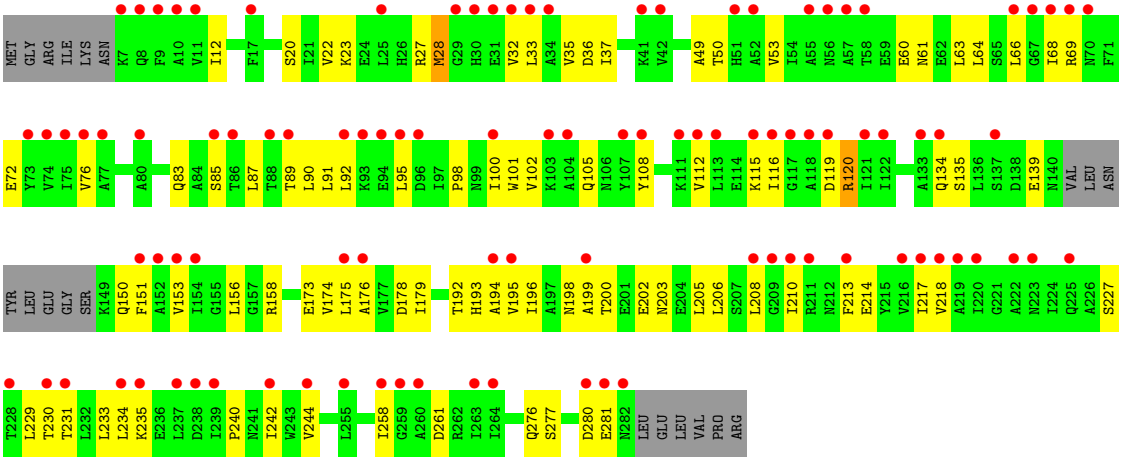
Chain B:





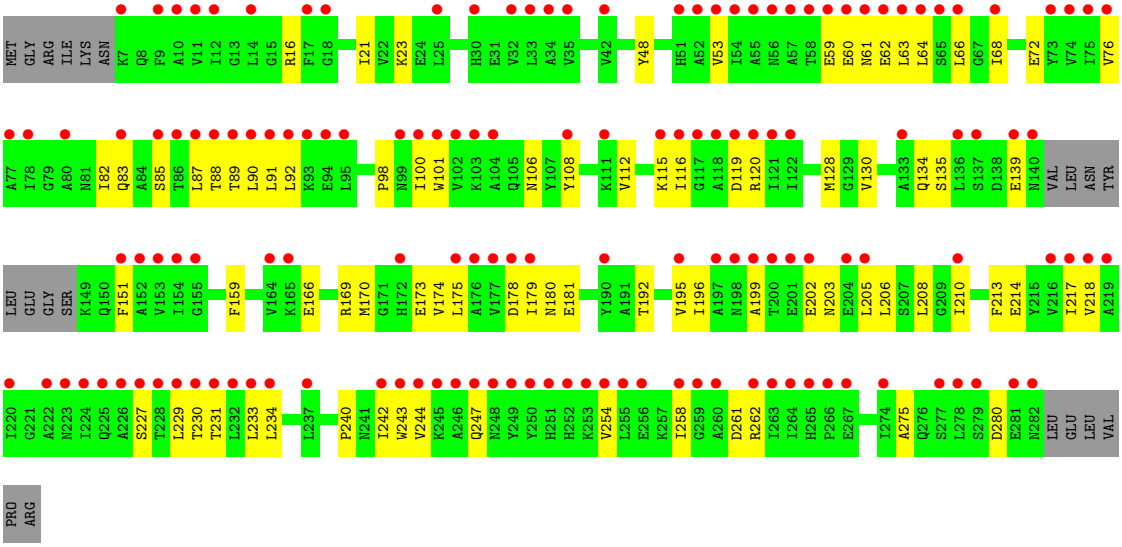
• Molecule 2: Ktr system potassium uptake protein A

Chain C:



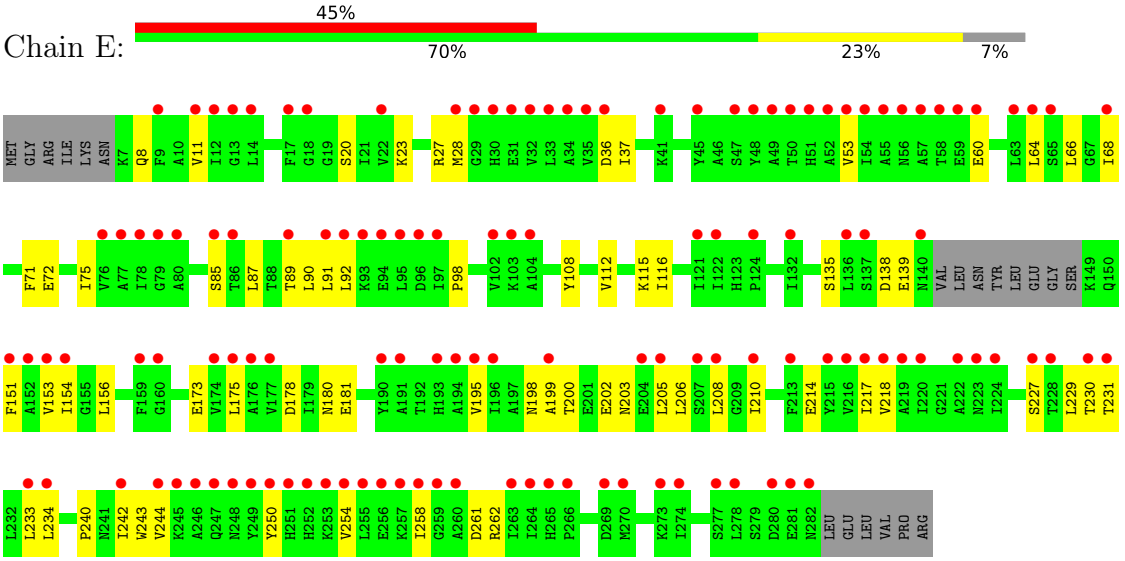
• Molecule 2: Ktr system potassium uptake protein A

Chain D:



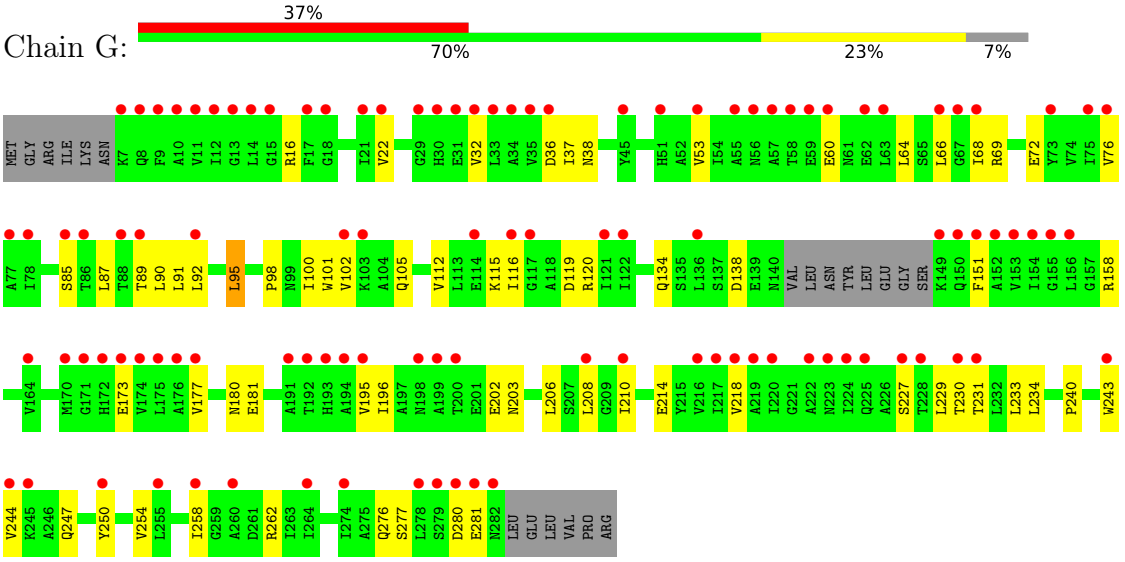
• Molecule 2: Ktr system potassium uptake protein A

Chain E:



• Molecule 2: Ktr system potassium uptake protein A

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.80Å 143.69Å 160.67Å 90.00° 112.37° 90.00°	Depositor
Resolution (Å)	48.00 – 5.77 48.89 – 5.77	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.00-5.77) 98.7 (48.89-5.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 5.73Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.405 , 0.426 0.404 , 0.417	Depositor DCC
R_{free} test set	1648 reflections (10.89%)	wwPDB-VP
Wilson B-factor (Å^2)	354.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 282.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	20736	wwPDB-VP
Average B, all atoms (Å^2)	362.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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	0.28	0/3157	0.50	0/4297
1	B	0.29	0/3157	0.51	0/4297
1	I	0.29	0/3157	0.50	0/4297
1	J	0.30	0/3157	0.51	0/4297
2	C	0.26	0/2130	0.46	0/2882
2	D	0.26	0/2130	0.46	0/2882
2	E	0.26	0/2130	0.46	0/2882
2	G	0.26	0/2130	0.46	0/2882
All	All	0.28	0/21148	0.49	0/28716

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3088	0	3227	129	0
1	B	3088	0	3227	127	0
1	I	3088	0	3227	109	0
1	J	3088	0	3227	123	0
2	C	2096	0	2120	68	0
2	D	2096	0	2120	58	0
2	E	2096	0	2120	48	0
2	G	2096	0	2120	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20736	0	21388	666	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 16.

All (666) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:278:THR:HA	1:I:391:VAL:HA	1.46	0.95
1:A:278:THR:HA	1:A:391:VAL:HA	1.51	0.93
1:J:278:THR:HA	1:J:391:VAL:HA	1.51	0.92
1:B:278:THR:HA	1:B:391:VAL:HA	1.60	0.83
1:J:61:THR:HG23	1:J:390:THR:HA	1.60	0.82
1:I:208:GLY:HA2	1:I:309:SER:H	1.46	0.80
1:I:309:SER:OG	1:I:310:THR:N	2.09	0.80
1:I:61:THR:HG23	1:I:390:THR:HA	1.63	0.78
1:A:208:GLY:HA2	1:A:309:SER:H	1.49	0.77
1:A:61:THR:HG23	1:A:390:THR:HA	1.67	0.76
1:B:61:THR:HG23	1:B:390:THR:HA	1.65	0.76
1:A:28:ILE:HG12	1:A:58:THR:HG21	1.67	0.75
1:I:28:ILE:HG12	1:I:58:THR:HG21	1.67	0.75
1:B:324:THR:HG21	1:B:338:ILE:HD11	1.68	0.74
2:D:134:GLN:NE2	2:D:170:MET:SD	2.60	0.73
1:I:304:GLY:HA3	1:I:312:SER:HB3	1.69	0.73
2:D:258:ILE:HD11	2:G:254:VAL:HG23	1.72	0.71
2:C:195:VAL:HG21	2:C:208:LEU:HD11	1.74	0.70
1:J:202:PHE:HE1	1:J:274:VAL:HG12	1.56	0.69
1:A:92:MET:HG2	1:A:133:LEU:HB2	1.74	0.69
2:C:90:LEU:HD21	2:D:115:LYS:HB2	1.73	0.69
1:J:43:LYS:HD3	1:B:42:THR:HG22	1.73	0.69
1:J:304:GLY:HA3	1:J:312:SER:HB3	1.74	0.69
2:G:181:GLU:HB3	2:G:196:ILE:HD13	1.74	0.69
1:I:304:GLY:N	1:I:314:ILE:O	2.26	0.69
2:E:53:VAL:HG21	2:E:66:LEU:HD11	1.75	0.69
1:J:28:ILE:HG12	1:J:58:THR:HG21	1.75	0.68
1:J:92:MET:HA	1:J:209:PHE:HE2	1.59	0.68
2:D:195:VAL:HG21	2:D:208:LEU:HD11	1.75	0.68
2:E:195:VAL:HG21	2:E:208:LEU:HD11	1.75	0.68
1:B:304:GLY:HA3	1:B:312:SER:HB3	1.76	0.68
2:C:53:VAL:HG21	2:C:66:LEU:HD11	1.77	0.67
2:C:115:LYS:HB2	2:D:90:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:MET:HA	1:J:209:PHE:CE2	2.30	0.67
1:B:250:GLU:OE2	1:B:293:THR:OG1	2.07	0.67
1:A:58:THR:HB	1:A:83:LEU:HG	1.76	0.67
1:A:257:LEU:O	1:A:259:HIS:N	2.27	0.67
1:B:304:GLY:N	1:B:314:ILE:O	2.25	0.66
2:E:208:LEU:HB3	2:E:210:ILE:HG13	1.77	0.66
1:I:257:LEU:HD13	1:I:268:ALA:HB3	1.76	0.66
1:J:304:GLY:N	1:J:314:ILE:O	2.26	0.66
1:B:133:LEU:O	1:B:137:SER:OG	2.12	0.66
2:E:66:LEU:HB3	2:E:68:ILE:HG13	1.78	0.66
2:G:53:VAL:HG21	2:G:66:LEU:HD11	1.78	0.66
2:G:105:GLN:O	2:G:158:ARG:NH1	2.29	0.66
1:B:301:MET:HB2	1:B:391:VAL:HG11	1.76	0.65
1:J:370:THR:HA	1:J:380:ILE:HD13	1.78	0.65
1:A:301:MET:HB2	1:A:391:VAL:HG11	1.78	0.65
1:B:171:SER:HB2	1:B:176:ALA:HB3	1.78	0.65
1:B:257:LEU:O	1:B:259:HIS:N	2.30	0.65
1:A:304:GLY:N	1:A:314:ILE:O	2.29	0.65
1:B:181:TRP:HE1	1:B:185:LEU:HA	1.61	0.65
2:C:20:SER:HA	2:C:23:LYS:HE2	1.78	0.65
1:J:301:MET:HB2	1:J:391:VAL:HG11	1.78	0.65
1:B:61:THR:HA	1:B:390:THR:HB	1.78	0.64
1:J:60:VAL:HG23	1:J:84:ILE:HG23	1.79	0.64
2:C:208:LEU:HB3	2:C:210:ILE:HG13	1.79	0.64
1:A:352:LEU:HD23	1:B:352:LEU:HD23	1.79	0.64
1:A:370:THR:HG23	1:A:380:ILE:HG21	1.79	0.64
1:I:150:ILE:HD11	1:I:162:LEU:HD23	1.79	0.63
1:J:72:PHE:HB3	1:J:76:GLY:HA3	1.81	0.63
1:A:150:ILE:HD11	1:A:162:LEU:HD23	1.81	0.63
2:C:105:GLN:O	2:C:158:ARG:NH1	2.31	0.63
1:B:409:ILE:HD13	1:B:412:ILE:HD12	1.81	0.63
2:E:20:SER:HA	2:E:23:LYS:HE2	1.80	0.63
1:B:28:ILE:HG12	1:B:58:THR:HG21	1.81	0.63
1:I:34:LEU:HB3	1:I:79:VAL:HG11	1.81	0.62
1:I:61:THR:HA	1:I:390:THR:HB	1.80	0.62
1:J:150:ILE:HD11	1:J:162:LEU:HD23	1.80	0.62
1:I:352:LEU:HD23	1:J:352:LEU:HD23	1.80	0.62
1:I:202:PHE:HE1	1:I:274:VAL:HG12	1.64	0.62
2:E:90:LEU:HD21	2:G:115:LYS:HB2	1.80	0.62
1:I:370:THR:HG23	1:I:380:ILE:HG21	1.82	0.62
2:G:195:VAL:HG21	2:G:208:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:O	1:A:251:TYR:HB2	1.99	0.62
1:J:171:SER:HB2	1:J:176:ALA:HB3	1.82	0.62
2:D:53:VAL:HG21	2:D:66:LEU:HD11	1.82	0.62
1:I:92:MET:HG2	1:I:133:LEU:HB2	1.81	0.62
1:J:140:ILE:HD12	1:J:143:ILE:HD11	1.82	0.62
1:A:189:VAL:HG11	1:A:260:LEU:HD21	1.82	0.62
1:B:140:ILE:HD12	1:B:143:ILE:HD11	1.82	0.61
1:B:150:ILE:HD11	1:B:162:LEU:HD23	1.81	0.61
1:A:434:ASN:HD22	2:G:203:ASN:HD22	1.47	0.61
1:A:304:GLY:HA3	1:A:312:SER:HB3	1.80	0.61
2:C:66:LEU:HB3	2:C:68:ILE:HG13	1.82	0.61
2:D:208:LEU:HB3	2:D:210:ILE:HG13	1.81	0.61
1:A:202:PHE:HE1	1:A:274:VAL:HG12	1.65	0.61
1:A:330:LEU:HD13	1:B:424:VAL:HG11	1.84	0.60
1:J:61:THR:HA	1:J:390:THR:HB	1.82	0.60
1:B:370:THR:HG23	1:B:380:ILE:HG21	1.83	0.60
1:A:307:SER:HA	1:A:315:LYS:HG3	1.83	0.60
2:G:69:ARG:HG2	2:G:95:LEU:HB3	1.84	0.60
1:B:210:THR:O	1:B:214:ASP:N	2.30	0.60
1:I:173:PHE:HB2	1:I:201:LEU:HD22	1.83	0.60
1:J:309:SER:OG	1:J:310:THR:N	2.33	0.60
1:B:60:VAL:HG23	1:B:84:ILE:HG23	1.84	0.60
1:I:60:VAL:HG23	1:I:84:ILE:HG23	1.83	0.60
1:A:140:ILE:HD12	1:A:143:ILE:HD11	1.84	0.59
1:I:94:PHE:HE1	1:I:422:THR:HG1	1.50	0.59
1:A:94:PHE:HE1	1:A:422:THR:HG1	1.49	0.59
1:A:61:THR:HA	1:A:390:THR:HB	1.85	0.59
1:I:370:THR:HA	1:I:380:ILE:HD13	1.84	0.58
1:B:272:GLN:OE1	1:B:284:LEU:N	2.37	0.58
1:J:202:PHE:CE1	1:J:274:VAL:HG12	2.37	0.58
1:B:309:SER:OG	1:B:310:THR:N	2.35	0.58
1:I:140:ILE:HD12	1:I:143:ILE:HD11	1.85	0.58
1:J:247:PHE:HE1	1:J:265:LYS:HB3	1.68	0.58
1:A:409:ILE:HD13	1:A:412:ILE:HD12	1.86	0.58
1:B:272:GLN:HA	1:B:275:THR:HG22	1.85	0.58
1:A:168:HIS:O	1:A:172:ALA:N	2.35	0.58
1:A:256:THR:HG22	1:A:257:LEU:H	1.69	0.58
2:C:76:VAL:HG21	2:C:89:THR:HG22	1.84	0.58
2:E:115:LYS:HB2	2:G:90:LEU:HD21	1.85	0.58
1:B:173:PHE:HB2	1:B:201:LEU:HD22	1.84	0.58
1:B:92:MET:HA	1:B:209:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:370:THR:HG23	1:J:380:ILE:HG21	1.86	0.57
1:B:227:HIS:CE1	1:B:317:THR:HG21	2.40	0.57
2:C:115:LYS:HD2	2:D:90:LEU:HG	1.85	0.57
2:D:180:ASN:OD1	2:D:181:GLU:N	2.32	0.57
1:B:322:ILE:HD13	1:B:355:SER:HB2	1.87	0.57
1:I:409:ILE:HD13	1:I:412:ILE:HD12	1.86	0.57
1:I:433:SER:HB2	1:J:333:LYS:HG2	1.86	0.57
1:J:246:VAL:HG11	1:J:272:GLN:HB3	1.86	0.57
1:B:247:PHE:O	1:B:251:TYR:HB2	2.05	0.57
1:B:92:MET:HA	1:B:209:PHE:HE2	1.70	0.57
1:J:208:GLY:HA2	1:J:309:SER:H	1.69	0.56
1:I:301:MET:HB2	1:I:391:VAL:HG11	1.87	0.56
2:D:66:LEU:HB3	2:D:68:ILE:HG13	1.85	0.56
1:J:379:GLN:HG3	1:J:395:MET:HB2	1.87	0.56
1:A:92:MET:HA	1:A:209:PHE:CE2	2.40	0.56
1:B:168:HIS:O	1:B:172:ALA:N	2.37	0.56
1:I:424:VAL:HG11	1:J:330:LEU:HD13	1.88	0.56
1:B:370:THR:HA	1:B:380:ILE:HD13	1.87	0.56
1:B:418:ILE:HG23	1:B:423:PHE:HB2	1.88	0.56
2:C:72:GLU:HA	2:C:98:PRO:HD2	1.87	0.56
1:A:294:ILE:HG23	1:A:382:PHE:HD2	1.71	0.56
1:A:322:ILE:HD13	1:A:355:SER:HB2	1.88	0.56
2:G:37:ILE:HG13	2:G:38:ASN:N	2.20	0.56
1:I:209:PHE:HA	1:I:212:LEU:HB2	1.87	0.56
1:I:256:THR:HB	1:I:284:LEU:HB3	1.87	0.56
1:J:145:ALA:HA	1:J:149:SER:HB2	1.88	0.56
2:C:175:LEU:HD21	2:C:208:LEU:HG	1.87	0.56
1:I:330:LEU:HD13	1:J:424:VAL:HG11	1.88	0.55
1:A:173:PHE:HB2	1:A:201:LEU:HD22	1.89	0.55
2:D:218:VAL:HB	2:D:244:VAL:HG13	1.87	0.55
1:A:370:THR:HA	1:A:380:ILE:HD13	1.88	0.55
1:B:72:PHE:HB3	1:B:76:GLY:HA3	1.89	0.55
1:B:202:PHE:HE1	1:B:274:VAL:HG12	1.70	0.55
2:C:258:ILE:HD11	2:E:254:VAL:HG23	1.87	0.55
2:D:181:GLU:HB3	2:D:196:ILE:HD13	1.88	0.55
1:J:210:THR:O	1:J:214:ASP:N	2.32	0.55
1:A:340:ARG:HD3	2:C:193:HIS:NE2	2.22	0.55
2:D:231:THR:HA	2:D:234:LEU:HD12	1.88	0.55
2:G:208:LEU:HB3	2:G:210:ILE:HG13	1.88	0.55
1:I:307:SER:HA	1:I:315:LYS:HG3	1.89	0.55
1:A:417:ARG:O	1:A:417:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:PHE:O	1:I:251:TYR:HB2	2.07	0.55
1:I:322:ILE:HD13	1:I:355:SER:HB2	1.89	0.55
1:J:168:HIS:O	1:J:172:ALA:N	2.37	0.55
2:G:101:TRP:CD2	2:G:120:ARG:HD3	2.41	0.55
1:J:344:LYS:HG3	1:J:346:PRO:HD2	1.88	0.55
1:A:145:ALA:HA	1:A:149:SER:HB2	1.88	0.55
1:B:294:ILE:HG23	1:B:382:PHE:HD2	1.72	0.54
1:J:398:THR:HA	1:J:401:LEU:HG	1.90	0.54
1:B:337:VAL:HA	1:B:342:SER:HA	1.90	0.54
1:I:67:ASP:O	1:I:71:GLN:HB3	2.07	0.54
1:I:227:HIS:CE1	1:I:317:THR:HG21	2.42	0.54
1:I:294:ILE:HG23	1:I:382:PHE:HD2	1.71	0.54
1:B:175:ASN:ND2	1:B:202:PHE:HB2	2.23	0.54
1:B:270:TYR:O	1:B:274:VAL:HG23	2.08	0.54
2:C:231:THR:HA	2:C:234:LEU:HD12	1.89	0.54
1:J:257:LEU:HD13	1:J:268:ALA:HB3	1.90	0.54
2:C:202:GLU:O	2:C:206:LEU:HG	2.08	0.54
1:J:303:ILE:HA	1:J:314:ILE:HG23	1.90	0.54
2:E:231:THR:HA	2:E:234:LEU:HD12	1.90	0.54
1:I:247:PHE:HE1	1:I:265:LYS:HB3	1.72	0.54
1:J:175:ASN:ND2	1:J:202:PHE:HB2	2.23	0.54
1:A:175:ASN:ND2	1:A:202:PHE:HB2	2.23	0.54
2:C:218:VAL:HB	2:C:244:VAL:HG13	1.90	0.54
1:A:209:PHE:HD1	1:A:212:LEU:HD12	1.73	0.53
2:D:218:VAL:HG21	2:D:231:THR:HG22	1.91	0.53
1:I:443:PHE:O	1:J:307:SER:OG	2.25	0.53
1:J:294:ILE:HG23	1:J:382:PHE:HD2	1.74	0.53
1:A:64:ALA:H	1:A:398:THR:HG21	1.74	0.53
1:A:247:PHE:HE1	1:A:265:LYS:HB3	1.72	0.53
1:A:344:LYS:HG3	1:A:346:PRO:HD2	1.91	0.53
1:A:146:LEU:HD13	1:A:166:LEU:HD23	1.90	0.53
1:A:204:THR:O	1:A:207:ILE:HG12	2.08	0.53
1:J:64:ALA:H	1:J:398:THR:HG21	1.73	0.53
1:A:60:VAL:HG12	1:A:84:ILE:HG23	1.88	0.53
1:B:257:LEU:O	1:B:260:LEU:N	2.34	0.53
2:C:33:LEU:HD21	2:C:66:LEU:HG	1.90	0.53
2:E:218:VAL:HG21	2:E:231:THR:HG22	1.90	0.53
1:I:227:HIS:HA	1:I:230:LEU:HD12	1.91	0.53
1:J:407:CYS:O	1:J:411:VAL:HG23	2.09	0.53
1:J:409:ILE:HD13	1:J:412:ILE:HD12	1.91	0.53
1:I:337:VAL:HA	1:I:342:SER:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:HB3	1:B:184:ASN:HA	1.92	0.52
1:J:95:ALA:HA	1:J:98:ILE:HB	1.91	0.52
2:E:202:GLU:O	2:E:206:LEU:HG	2.09	0.52
1:I:73:THR:HG22	1:I:74:VAL:H	1.75	0.52
2:D:89:THR:HA	2:D:92:LEU:HD12	1.91	0.52
2:D:181:GLU:CB	2:D:196:ILE:HD13	2.40	0.52
1:I:209:PHE:HD1	1:I:212:LEU:HD12	1.74	0.52
1:I:204:THR:O	1:I:207:ILE:HG12	2.10	0.52
1:I:256:THR:HB	1:I:284:LEU:HD13	1.91	0.52
2:D:151:PHE:HB2	2:D:173:GLU:O	2.10	0.52
1:I:146:LEU:HD13	1:I:166:LEU:HD23	1.92	0.52
1:I:92:MET:HA	1:I:209:PHE:CE2	2.45	0.51
1:J:67:ASP:O	1:J:71:GLN:HB3	2.10	0.51
1:A:270:TYR:O	1:A:274:VAL:HG23	2.10	0.51
1:B:314:ILE:HD12	1:B:355:SER:HA	1.92	0.51
1:B:204:THR:O	1:B:207:ILE:HG12	2.11	0.51
2:C:90:LEU:HG	2:D:115:LYS:HD2	1.91	0.51
1:A:350:LYS:HE3	1:A:421:LEU:HD12	1.91	0.51
1:A:424:VAL:HG11	1:B:330:LEU:HD13	1.92	0.51
2:D:227:SER:O	2:D:231:THR:HG23	2.10	0.51
2:G:16:ARG:NH1	2:G:247:GLN:O	2.43	0.51
1:A:227:HIS:HA	1:A:230:LEU:HD12	1.92	0.51
1:B:67:ASP:O	1:B:71:GLN:HB3	2.09	0.51
2:C:192:THR:HG22	2:C:193:HIS:HD1	1.75	0.51
2:G:69:ARG:HD3	2:G:95:LEU:HD12	1.92	0.51
2:G:202:GLU:O	2:G:206:LEU:HG	2.10	0.51
1:A:67:ASP:O	1:A:71:GLN:HB3	2.10	0.51
2:E:87:LEU:O	2:E:91:LEU:HG	2.11	0.51
1:I:92:MET:HG2	1:I:133:LEU:HD13	1.93	0.51
1:I:168:HIS:O	1:I:172:ALA:N	2.42	0.51
1:J:227:HIS:HA	1:J:230:LEU:HD12	1.92	0.51
2:D:169:ARG:NH1	2:D:170:MET:HG2	2.25	0.51
1:A:171:SER:HB2	1:A:176:ALA:HB3	1.93	0.51
1:B:208:GLY:HA2	1:B:309:SER:H	1.76	0.51
1:B:294:ILE:HG23	1:B:382:PHE:CD2	2.46	0.51
1:I:302:PHE:HB2	1:I:385:PHE:HD2	1.76	0.51
1:B:42:THR:OG1	1:B:43:LYS:N	2.43	0.51
2:G:66:LEU:HB3	2:G:68:ILE:HG13	1.92	0.51
2:G:277:SER:O	2:G:281:GLU:HB2	2.10	0.51
1:J:257:LEU:HD11	1:J:265:LYS:HA	1.92	0.51
1:A:337:VAL:HA	1:A:342:SER:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:227:SER:O	2:E:231:THR:HG23	2.11	0.51
1:J:146:LEU:HD13	1:J:166:LEU:HD23	1.92	0.51
1:B:379:GLN:HA	1:B:395:MET:HE3	1.93	0.51
2:D:23:LYS:HG2	2:D:48:TYR:HD2	1.76	0.51
2:D:101:TRP:CD2	2:D:120:ARG:HD3	2.45	0.51
2:E:218:VAL:HB	2:E:244:VAL:HG13	1.93	0.50
2:C:60:GLU:O	2:C:64:LEU:HG	2.11	0.50
1:I:314:ILE:HD12	1:I:355:SER:HA	1.93	0.50
1:J:61:THR:HG21	1:J:413:MET:HG2	1.93	0.50
2:C:85:SER:O	2:C:89:THR:HG23	2.11	0.50
1:J:173:PHE:HB2	1:J:201:LEU:HD22	1.93	0.50
1:B:64:ALA:H	1:B:398:THR:HG21	1.77	0.50
1:B:227:HIS:HA	1:B:230:LEU:HD12	1.93	0.50
2:E:151:PHE:HB2	2:E:173:GLU:O	2.12	0.50
2:D:214:GLU:HA	2:D:240:PRO:HD2	1.93	0.50
1:J:247:PHE:O	1:J:251:TYR:HB2	2.11	0.49
2:E:180:ASN:OD1	2:E:181:GLU:N	2.42	0.49
1:J:63:LEU:HB3	1:J:398:THR:HG21	1.94	0.49
1:B:81:MET:SD	1:B:167:PHE:HA	2.52	0.49
2:C:218:VAL:HG21	2:C:231:THR:HG22	1.93	0.49
1:I:417:ARG:O	1:I:417:ARG:NH1	2.45	0.49
1:A:209:PHE:HA	1:A:212:LEU:HB2	1.93	0.49
2:E:214:GLU:HA	2:E:240:PRO:HD2	1.94	0.49
1:I:294:ILE:HG23	1:I:382:PHE:CD2	2.47	0.49
1:J:174:ASN:HA	1:J:310:THR:HG21	1.95	0.49
2:C:242:ILE:HG13	2:C:261:ASP:H	1.78	0.49
2:D:100:ILE:HG13	2:D:119:ASP:H	1.76	0.49
1:A:294:ILE:HG23	1:A:382:PHE:CD2	2.48	0.49
1:A:303:ILE:HA	1:A:314:ILE:HG23	1.94	0.49
1:I:60:VAL:O	1:I:60:VAL:HG13	2.12	0.49
1:I:303:ILE:HA	1:I:314:ILE:HG23	1.95	0.49
2:D:60:GLU:O	2:D:64:LEU:HG	2.13	0.49
2:D:85:SER:O	2:D:89:THR:HG23	2.13	0.49
2:E:156:LEU:N	2:E:178:ASP:OD2	2.37	0.49
1:I:175:ASN:ND2	1:I:310:THR:OG1	2.46	0.49
1:I:270:TYR:O	1:I:274:VAL:HG23	2.12	0.49
1:J:272:GLN:HE22	1:J:284:LEU:HB2	1.78	0.49
1:J:322:ILE:HD13	1:J:355:SER:HB2	1.94	0.49
2:E:229:LEU:O	2:E:233:LEU:HG	2.12	0.49
1:J:37:LEU:O	1:J:41:THR:HG22	2.12	0.48
1:A:209:PHE:CD2	1:A:308:ALA:HB1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ILE:HG23	1:A:423:PHE:HB2	1.94	0.48
1:B:203:ILE:HD11	1:B:274:VAL:HG11	1.96	0.48
2:D:112:VAL:O	2:D:116:ILE:HG12	2.13	0.48
2:D:243:TRP:CE2	2:D:262:ARG:HG3	2.48	0.48
1:I:418:ILE:HG23	1:I:423:PHE:HB2	1.95	0.48
1:A:434:ASN:ND2	2:G:203:ASN:HD22	2.11	0.48
2:D:72:GLU:HA	2:D:98:PRO:HD2	1.96	0.48
1:J:20:LEU:HD13	1:J:94:PHE:HE1	1.78	0.48
1:J:199:THR:HG21	1:J:270:TYR:HE2	1.78	0.48
1:J:294:ILE:HG23	1:J:382:PHE:CD2	2.49	0.48
1:A:379:GLN:HG3	1:A:395:MET:HB2	1.95	0.48
1:B:421:LEU:HD23	1:B:421:LEU:HA	1.70	0.48
2:C:83:GLN:NE2	2:D:108:TYR:HB2	2.29	0.48
2:C:112:VAL:O	2:C:116:ILE:HG12	2.14	0.48
2:G:243:TRP:CE2	2:G:262:ARG:HG3	2.49	0.48
1:I:129:LEU:HG	1:I:133:LEU:HD23	1.95	0.48
1:J:354:VAL:HG13	1:J:420:PRO:HG2	1.96	0.48
1:B:303:ILE:HA	1:B:314:ILE:HG23	1.96	0.48
1:J:81:MET:SD	1:J:170:ILE:HD12	2.53	0.48
1:B:322:ILE:CD1	1:B:355:SER:HB2	2.43	0.48
1:B:436:ARG:HB2	2:C:196:ILE:HB	1.96	0.48
1:A:227:HIS:CE1	1:A:317:THR:HG21	2.48	0.48
2:G:227:SER:O	2:G:231:THR:HG23	2.14	0.48
1:B:20:LEU:HD13	1:B:94:PHE:HE1	1.78	0.48
2:C:87:LEU:O	2:C:91:LEU:HG	2.14	0.48
1:J:81:MET:SD	1:J:167:PHE:HA	2.54	0.47
1:A:188:TYR:CG	1:A:194:VAL:HG21	2.49	0.47
1:A:268:ALA:HB1	1:A:284:LEU:HD11	1.96	0.47
1:B:146:LEU:HD13	1:B:166:LEU:HD23	1.94	0.47
1:B:407:CYS:O	1:B:411:VAL:HG23	2.14	0.47
1:B:438:PRO:HD3	2:C:194:ALA:O	2.14	0.47
2:D:202:GLU:O	2:D:206:LEU:HG	2.13	0.47
2:E:72:GLU:HA	2:E:98:PRO:HD2	1.96	0.47
2:C:198:ASN:OD1	2:C:200:THR:OG1	2.21	0.47
2:G:36:ASP:OD1	2:G:37:ILE:N	2.47	0.47
1:B:60:VAL:HG22	1:B:176:ALA:HA	1.95	0.47
2:D:76:VAL:HG21	2:D:89:THR:HG22	1.96	0.47
2:D:87:LEU:O	2:D:91:LEU:HG	2.14	0.47
2:E:27:ARG:HH12	2:E:28:MET:HG2	1.80	0.47
2:G:254:VAL:O	2:G:258:ILE:HG12	2.15	0.47
1:J:418:ILE:HG23	1:J:423:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PHE:HE1	1:B:265:LYS:HB3	1.79	0.47
2:G:250:TYR:O	2:G:254:VAL:HG12	2.15	0.47
1:B:73:THR:HG22	1:B:74:VAL:H	1.79	0.47
1:I:208:GLY:HA2	1:I:308:ALA:HB3	1.97	0.47
1:I:407:CYS:O	1:I:411:VAL:HG23	2.15	0.47
1:J:29:ILE:HD13	1:J:51:LEU:HD11	1.96	0.47
1:A:34:LEU:HB3	1:A:79:VAL:HG11	1.96	0.47
1:A:296:PHE:HB2	1:B:367:PHE:CE2	2.50	0.47
1:B:92:MET:SD	1:B:133:LEU:HB2	2.55	0.47
1:B:323:LEU:O	1:B:327:ILE:HG13	2.15	0.47
2:C:76:VAL:HB	2:C:102:VAL:HG13	1.96	0.47
2:C:89:THR:HA	2:C:92:LEU:HD12	1.95	0.47
2:C:108:TYR:HB2	2:D:83:GLN:NE2	2.30	0.47
2:C:150:GLN:HG3	2:C:213:PHE:CE2	2.49	0.47
1:J:153:VAL:N	1:J:154:PRO:CD	2.78	0.47
1:J:208:GLY:HA2	1:J:308:ALA:HB3	1.97	0.47
1:B:46:SER:HB3	1:B:48:ILE:HD12	1.96	0.47
1:B:81:MET:SD	1:B:170:ILE:HD12	2.54	0.47
2:G:180:ASN:OD1	2:G:181:GLU:N	2.44	0.47
1:J:204:THR:O	1:J:207:ILE:HG12	2.14	0.47
1:J:302:PHE:HB2	1:J:385:PHE:HD2	1.80	0.47
2:C:227:SER:O	2:C:231:THR:HG23	2.15	0.47
2:E:202:GLU:HG2	2:E:203:ASN:N	2.30	0.47
1:A:208:GLY:HA2	1:A:308:ALA:HB3	1.95	0.47
1:I:257:LEU:HD11	1:I:265:LYS:HA	1.96	0.46
1:A:443:PHE:O	1:B:307:SER:OG	2.32	0.46
1:B:133:LEU:HD12	1:B:134:PHE:N	2.30	0.46
2:C:22:VAL:HG13	2:C:49:ALA:HB2	1.97	0.46
2:G:76:VAL:HB	2:G:102:VAL:HG13	1.97	0.46
1:B:175:ASN:HB3	1:B:278:THR:O	2.14	0.46
2:C:135:SER:O	2:C:139:GLU:HB2	2.16	0.46
2:C:214:GLU:HA	2:C:240:PRO:HD2	1.97	0.46
1:I:64:ALA:H	1:I:398:THR:HG21	1.79	0.46
1:I:379:GLN:HE21	1:I:397:LEU:HB2	1.80	0.46
1:A:46:SER:HB3	1:A:48:ILE:HD12	1.97	0.46
1:A:199:THR:HA	1:A:202:PHE:CE2	2.50	0.46
1:I:318:THR:HG22	1:I:322:ILE:HD11	1.98	0.46
1:I:323:LEU:O	1:I:327:ILE:HG13	2.15	0.46
1:A:63:LEU:HB3	1:A:398:THR:HG21	1.96	0.46
1:A:253:ASN:HD22	1:A:290:ARG:HG3	1.79	0.46
1:A:153:VAL:N	1:A:154:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LEU:HA	1:B:260:LEU:HD13	1.98	0.46
2:D:178:ASP:OD1	2:D:179:ILE:N	2.48	0.46
1:I:322:ILE:CD1	1:I:355:SER:HB2	2.46	0.46
2:E:60:GLU:O	2:E:64:LEU:HG	2.16	0.46
1:J:314:ILE:HD12	1:J:355:SER:HA	1.97	0.46
1:B:145:ALA:HB2	1:B:169:ALA:CB	2.46	0.46
1:B:199:THR:HG21	1:B:270:TYR:HE2	1.81	0.46
1:B:379:GLN:HG3	1:B:395:MET:HB2	1.96	0.46
2:C:100:ILE:HG13	2:C:119:ASP:H	1.80	0.46
1:J:91:PHE:HB2	1:J:417:ARG:NH2	2.31	0.46
2:E:89:THR:HA	2:E:92:LEU:HD12	1.97	0.46
1:I:153:VAL:N	1:I:154:PRO:CD	2.79	0.46
1:J:133:LEU:HD12	1:J:134:PHE:N	2.31	0.46
1:J:145:ALA:HB2	1:J:169:ALA:CB	2.45	0.46
2:C:202:GLU:HG2	2:C:203:ASN:N	2.31	0.46
1:A:208:GLY:CA	1:A:308:ALA:HB3	2.46	0.46
1:B:306:GLY:O	1:B:309:SER:HB3	2.16	0.46
1:B:437:TYR:HB3	1:B:438:PRO:HD2	1.98	0.46
2:C:199:ALA:HA	2:C:205:LEU:HD11	1.98	0.46
2:G:89:THR:HA	2:G:92:LEU:HD12	1.98	0.46
1:I:133:LEU:HD12	1:I:134:PHE:N	2.31	0.45
1:I:199:THR:HA	1:I:202:PHE:CE2	2.51	0.45
1:J:60:VAL:O	1:J:60:VAL:HG13	2.15	0.45
1:J:242:ALA:CB	1:J:273:ALA:HB1	2.46	0.45
1:B:153:VAL:N	1:B:154:PRO:CD	2.79	0.45
1:B:209:PHE:H	1:B:308:ALA:HB3	1.81	0.45
1:B:417:ARG:O	1:B:417:ARG:NH1	2.49	0.45
2:G:87:LEU:O	2:G:91:LEU:HG	2.16	0.45
1:J:36:MET:HA	1:J:45:LEU:HD23	1.96	0.45
1:A:442:VAL:HG13	1:B:347:ILE:HG21	1.99	0.45
1:B:272:GLN:HE22	1:B:284:LEU:HD12	1.80	0.45
2:G:112:VAL:O	2:G:116:ILE:HG12	2.16	0.45
1:I:171:SER:HB3	1:I:176:ALA:HB3	1.97	0.45
1:J:172:ALA:O	1:J:202:PHE:HB3	2.16	0.45
1:J:257:LEU:HA	1:J:260:LEU:HD22	1.97	0.45
1:A:150:ILE:O	1:A:154:PRO:HD3	2.17	0.45
1:A:437:TYR:N	2:G:196:ILE:HD12	2.31	0.45
2:E:242:ILE:HG13	2:E:261:ASP:H	1.82	0.45
1:J:46:SER:HB3	1:J:48:ILE:HD12	1.98	0.45
2:G:151:PHE:HB2	2:G:173:GLU:O	2.16	0.45
1:I:91:PHE:HB2	1:I:417:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:199:THR:HG21	1:J:270:TYR:CE2	2.51	0.45
1:A:421:LEU:HD21	1:B:329:TYR:CE1	2.51	0.45
1:I:175:ASN:OD1	1:I:202:PHE:HB2	2.16	0.45
1:A:353:ALA:O	1:A:357:THR:OG1	2.23	0.45
1:A:366:ILE:HD13	1:A:381:VAL:HG13	1.99	0.45
1:B:199:THR:HA	1:B:202:PHE:CE2	2.52	0.45
2:D:130:VAL:HB	2:D:166:GLU:HG3	1.98	0.45
2:G:100:ILE:HG13	2:G:119:ASP:H	1.80	0.45
1:A:327:ILE:O	1:A:331:ARG:HG3	2.16	0.45
1:B:350:LYS:HE3	1:B:421:LEU:HD12	1.98	0.45
2:D:230:THR:O	2:D:234:LEU:HG	2.17	0.45
1:J:227:HIS:CE1	1:J:317:THR:HG21	2.51	0.45
1:A:94:PHE:HE1	1:A:422:THR:OG1	2.00	0.45
1:B:319:PHE:CZ	1:B:323:LEU:HD22	2.52	0.45
2:D:242:ILE:HG13	2:D:261:ASP:H	1.82	0.45
1:J:92:MET:SD	1:J:133:LEU:HB2	2.57	0.45
1:J:226:LEU:O	1:J:230:LEU:HG	2.17	0.45
1:A:398:THR:HA	1:A:401:LEU:HG	1.99	0.45
1:B:256:THR:HG22	1:B:289:MET:HG2	1.97	0.45
2:C:69:ARG:HG2	2:C:95:LEU:HB3	1.98	0.45
2:G:60:GLU:O	2:G:64:LEU:HG	2.17	0.45
1:I:378:LEU:HG	1:I:395:MET:HE1	1.99	0.44
1:A:378:LEU:HG	1:A:395:MET:HE1	1.98	0.44
2:E:135:SER:O	2:E:139:GLU:HB2	2.18	0.44
2:E:250:TYR:O	2:E:254:VAL:HG12	2.17	0.44
1:I:301:MET:HB2	1:I:391:VAL:HG21	1.99	0.44
1:J:209:PHE:H	1:J:308:ALA:HB3	1.82	0.44
1:J:323:LEU:O	1:J:327:ILE:HG13	2.17	0.44
1:A:316:LEU:O	1:A:320:ILE:HG13	2.16	0.44
1:J:133:LEU:O	1:J:137:SER:OG	2.33	0.44
1:J:206:GLY:HA2	1:J:310:THR:OG1	2.16	0.44
2:E:230:THR:O	2:E:234:LEU:HG	2.18	0.44
2:C:277:SER:O	2:C:281:GLU:HB2	2.17	0.44
2:G:231:THR:HA	2:G:234:LEU:HD12	1.99	0.44
1:I:210:THR:O	1:I:214:ASP:N	2.41	0.44
1:J:91:PHE:HE2	1:J:308:ALA:HB1	1.83	0.44
1:I:379:GLN:NE2	1:I:397:LEU:HB2	2.32	0.44
1:J:337:VAL:HA	1:J:342:SER:HA	1.99	0.44
2:D:229:LEU:O	2:D:233:LEU:HG	2.18	0.44
1:A:61:THR:HG21	1:A:413:MET:HG2	1.99	0.44
1:A:296:PHE:HB2	1:B:367:PHE:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:PRO:O	1:B:20:LEU:HG	2.17	0.44
2:C:27:ARG:HH12	2:C:28:MET:HG2	1.81	0.44
2:D:21:ILE:HG13	2:D:275:ALA:HB2	1.99	0.44
2:D:135:SER:O	2:D:139:GLU:HB2	2.17	0.44
1:A:179:SER:HB3	1:A:184:ASN:HA	1.99	0.44
1:A:436:ARG:HA	1:A:436:ARG:HD3	1.87	0.44
2:G:72:GLU:N	2:G:72:GLU:OE1	2.50	0.44
1:I:29:ILE:HD13	1:I:51:LEU:HD11	1.99	0.44
1:I:305:ALA:O	1:I:309:SER:HB2	2.18	0.44
1:J:60:VAL:HG22	1:J:176:ALA:HA	1.99	0.44
1:J:322:ILE:CD1	1:J:355:SER:HB2	2.48	0.44
1:J:353:ALA:O	1:J:357:THR:OG1	2.27	0.44
1:A:210:THR:O	1:A:214:ASP:N	2.46	0.44
1:A:286:PHE:CZ	1:A:393:LEU:HG	2.53	0.44
1:B:189:VAL:HG11	1:B:260:LEU:HD21	2.00	0.44
2:D:59:GLU:HB2	2:D:62:GLU:HG3	1.99	0.44
2:E:199:ALA:HB1	2:E:230:THR:HG23	2.00	0.44
1:J:179:SER:HB3	1:J:184:ASN:HA	1.99	0.43
1:J:294:ILE:O	1:J:298:LEU:HD13	2.18	0.43
1:J:377:PHE:O	1:J:381:VAL:HG23	2.18	0.43
1:J:378:LEU:HG	1:J:395:MET:HE1	2.00	0.43
2:C:214:GLU:OE1	2:C:214:GLU:N	2.48	0.43
2:E:112:VAL:O	2:E:116:ILE:HG12	2.17	0.43
1:A:322:ILE:CD1	1:A:355:SER:HB2	2.48	0.43
2:C:60:GLU:HG2	2:C:61:ASN:N	2.33	0.43
1:I:208:GLY:CA	1:I:308:ALA:HB3	2.48	0.43
1:I:276:PRO:HB2	1:I:300:LEU:HG	2.01	0.43
1:A:145:ALA:HB2	1:A:169:ALA:CB	2.48	0.43
1:A:189:VAL:CG1	1:A:260:LEU:HD21	2.47	0.43
1:A:203:ILE:O	1:A:207:ILE:HG23	2.18	0.43
1:B:226:LEU:O	1:B:230:LEU:HG	2.18	0.43
1:B:322:ILE:HD11	1:B:351:ALA:O	2.18	0.43
2:C:153:VAL:HG22	2:C:217:ILE:HB	2.00	0.43
2:C:156:LEU:HD21	2:C:176:ALA:HB1	1.99	0.43
2:D:205:LEU:HA	2:D:210:ILE:HD12	2.00	0.43
1:I:203:ILE:O	1:I:207:ILE:HG23	2.18	0.43
1:A:177:GLY:HA3	1:A:280:GLY:HA3	1.99	0.43
1:A:268:ALA:O	1:A:272:GLN:HB2	2.18	0.43
2:C:101:TRP:CD2	2:C:120:ARG:HD2	2.53	0.43
2:E:243:TRP:CE2	2:E:262:ARG:HG3	2.53	0.43
2:G:85:SER:O	2:G:89:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:202:GLU:HG2	2:G:203:ASN:N	2.33	0.43
1:A:373:GLU:OE2	1:A:402:THR:N	2.48	0.43
2:C:178:ASP:OD1	2:C:179:ILE:N	2.51	0.43
2:D:174:VAL:H	2:D:192:THR:HB	1.83	0.43
2:E:205:LEU:HA	2:E:210:ILE:HD12	2.01	0.43
2:G:214:GLU:HA	2:G:240:PRO:HD2	1.99	0.43
1:I:60:VAL:HG22	1:I:176:ALA:HA	2.00	0.43
1:I:146:LEU:HD12	1:I:146:LEU:HA	1.89	0.43
1:I:81:MET:HG3	1:I:170:ILE:HD12	2.00	0.43
1:J:388:PHE:O	1:J:416:GLY:HA3	2.18	0.43
1:J:390:THR:HG21	1:J:417:ARG:HB2	2.01	0.43
1:A:73:THR:HG22	1:A:74:VAL:H	1.83	0.43
1:A:199:THR:HG21	1:A:270:TYR:HE2	1.82	0.43
1:A:203:ILE:HD11	1:A:274:VAL:HG11	1.99	0.43
1:B:150:ILE:O	1:B:154:PRO:HD3	2.19	0.43
1:B:388:PHE:O	1:B:416:GLY:HA3	2.19	0.43
2:C:208:LEU:HD23	2:C:210:ILE:HD11	2.00	0.43
1:I:244:LEU:O	1:I:248:ILE:HG12	2.17	0.43
1:I:417:ARG:HA	1:I:417:ARG:HD2	1.87	0.43
1:J:297:THR:HA	1:J:300:LEU:HB3	2.01	0.43
1:A:294:ILE:O	1:A:298:LEU:HD13	2.19	0.43
1:B:316:LEU:O	1:B:320:ILE:HG13	2.18	0.43
2:C:27:ARG:NH1	2:C:28:MET:HG2	2.34	0.43
2:C:174:VAL:H	2:C:192:THR:HB	1.84	0.43
2:D:199:ALA:HB1	2:D:230:THR:HG23	2.00	0.43
2:E:217:ILE:HA	2:E:243:TRP:O	2.19	0.43
1:I:92:MET:HG3	1:I:133:LEU:HD22	2.01	0.43
1:J:62:GLY:HA3	1:J:392:GLY:HA2	2.01	0.43
1:A:60:VAL:CG1	1:A:84:ILE:HG23	2.49	0.43
1:A:382:PHE:HE1	1:A:393:LEU:O	2.02	0.43
2:G:72:GLU:HA	2:G:98:PRO:HD2	2.00	0.43
1:I:94:PHE:HE1	1:I:422:THR:OG1	2.00	0.43
1:A:40:SER:HB3	1:A:75:PHE:CD2	2.54	0.43
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.90	0.43
1:A:257:LEU:O	1:A:260:LEU:N	2.39	0.43
1:J:369:LEU:HD11	1:J:409:ILE:HD11	2.01	0.42
1:A:302:PHE:HB2	1:A:385:PHE:HD2	1.83	0.42
1:B:63:LEU:HB3	1:B:398:THR:HG21	2.00	0.42
1:B:320:ILE:O	1:B:324:THR:HG22	2.18	0.42
2:C:63:LEU:HG	2:C:68:ILE:HD12	2.01	0.42
1:A:307:SER:HA	1:A:315:LYS:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:SER:HB3	1:B:75:PHE:CD2	2.54	0.42
2:C:72:GLU:OE1	2:C:72:GLU:N	2.51	0.42
1:I:316:LEU:O	1:I:320:ILE:HG13	2.18	0.42
1:I:322:ILE:HD11	1:I:351:ALA:O	2.19	0.42
1:J:383:GLU:HG3	1:J:397:LEU:HD23	2.01	0.42
1:B:418:ILE:CG2	1:B:423:PHE:HB2	2.49	0.42
2:C:229:LEU:O	2:C:233:LEU:HG	2.18	0.42
2:E:66:LEU:HD12	2:E:66:LEU:HA	1.91	0.42
1:A:407:CYS:O	1:A:411:VAL:HG23	2.20	0.42
1:B:294:ILE:O	1:B:298:LEU:HD13	2.20	0.42
2:C:151:PHE:HB2	2:C:173:GLU:O	2.20	0.42
2:D:60:GLU:HG2	2:D:61:ASN:N	2.34	0.42
2:E:198:ASN:HD21	2:E:200:THR:HG23	1.84	0.42
1:I:153:VAL:N	1:I:154:PRO:HD2	2.35	0.42
1:I:388:PHE:O	1:I:416:GLY:HA3	2.18	0.42
1:J:306:GLY:O	1:J:309:SER:HB3	2.18	0.42
1:I:424:VAL:HG11	1:J:330:LEU:HD22	2.00	0.42
1:B:95:ALA:HA	1:B:98:ILE:HB	2.00	0.42
2:C:36:ASP:OD1	2:C:37:ILE:N	2.52	0.42
1:I:188:TYR:CG	1:I:194:VAL:HG21	2.55	0.42
1:J:256:THR:HB	1:J:284:LEU:HB3	2.01	0.42
1:B:37:LEU:O	1:B:41:THR:HG22	2.19	0.42
1:B:42:THR:HG23	1:B:71:GLN:O	2.20	0.42
1:B:215:VAL:HG22	1:B:224:PHE:CE2	2.55	0.42
1:I:226:LEU:O	1:I:230:LEU:HG	2.20	0.42
1:J:199:THR:HA	1:J:202:PHE:CE2	2.55	0.42
1:A:148:LEU:HG	1:A:151:ARG:CZ	2.50	0.42
1:A:251:TYR:O	1:A:258:GLY:HA2	2.19	0.42
1:A:367:PHE:HE2	1:B:296:PHE:HB2	1.84	0.42
1:B:322:ILE:O	1:B:326:VAL:HG23	2.19	0.42
2:C:32:VAL:H	2:C:50:THR:HB	1.83	0.42
2:E:199:ALA:HA	2:E:205:LEU:HD11	2.02	0.42
1:I:204:THR:O	1:I:212:LEU:HD21	2.20	0.42
1:I:291:GLU:O	1:I:295:VAL:HG23	2.20	0.42
1:J:436:ARG:HA	1:J:436:ARG:HD3	1.90	0.42
1:A:133:LEU:HD12	1:A:134:PHE:N	2.35	0.42
2:E:72:GLU:N	2:E:72:GLU:OE1	2.52	0.42
2:E:153:VAL:HG22	2:E:217:ILE:HB	2.01	0.42
2:E:11:VAL:HG22	2:E:75:ILE:HB	2.02	0.42
2:E:254:VAL:O	2:E:258:ILE:HG12	2.19	0.42
1:I:40:SER:HB3	1:I:75:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:317:THR:HA	1:I:320:ILE:HD12	2.02	0.41
2:C:83:GLN:HE22	2:D:106:ASN:ND2	2.18	0.41
2:D:128:MET:HG3	2:D:159:PHE:HE1	1.85	0.41
2:D:202:GLU:HG2	2:D:203:ASN:N	2.34	0.41
2:E:154:ILE:N	2:E:217:ILE:O	2.33	0.41
1:J:230:LEU:HD23	1:J:339:PHE:CE2	2.56	0.41
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.59	0.41
1:B:354:VAL:HG13	1:B:420:PRO:HG2	2.02	0.41
2:C:156:LEU:N	2:C:178:ASP:OD2	2.48	0.41
2:D:217:ILE:HA	2:D:243:TRP:O	2.20	0.41
2:D:254:VAL:O	2:D:258:ILE:HG12	2.19	0.41
2:E:27:ARG:NH1	2:E:28:MET:HG2	2.35	0.41
1:I:91:PHE:HD1	1:I:91:PHE:HA	1.70	0.41
1:I:379:GLN:HG3	1:I:395:MET:HB2	2.02	0.41
1:J:204:THR:O	1:J:212:LEU:HD21	2.21	0.41
1:B:244:LEU:O	1:B:248:ILE:HG12	2.20	0.41
2:C:83:GLN:OE1	2:D:82:ILE:HD13	2.20	0.41
2:C:230:THR:O	2:C:234:LEU:HG	2.20	0.41
2:E:36:ASP:OD1	2:E:37:ILE:N	2.54	0.41
1:J:89:LEU:HA	1:J:92:MET:HG3	2.01	0.41
1:J:302:PHE:HZ	1:J:358:SER:HG	1.65	0.41
1:B:91:PHE:CD1	1:B:310:THR:HA	2.56	0.41
1:B:145:ALA:HB2	1:B:169:ALA:HB3	2.02	0.41
1:J:203:ILE:HD11	1:J:274:VAL:HG11	2.02	0.41
1:I:48:ILE:HG22	1:I:406:LYS:HD3	2.02	0.41
1:J:148:LEU:HG	1:J:151:ARG:CZ	2.51	0.41
1:J:242:ALA:HB1	1:J:273:ALA:HB1	2.01	0.41
1:A:209:PHE:H	1:A:308:ALA:HB3	1.85	0.41
1:A:272:GLN:OE1	1:A:283:SER:HB3	2.20	0.41
1:B:327:ILE:O	1:B:331:ARG:HG3	2.21	0.41
2:D:175:LEU:HD22	2:D:213:PHE:CE1	2.56	0.41
1:J:45:LEU:HG	1:J:50:ALA:HB2	2.02	0.41
1:J:322:ILE:O	1:J:326:VAL:HG23	2.20	0.41
1:A:188:TYR:CD1	1:A:194:VAL:HG21	2.56	0.41
1:A:209:PHE:HA	1:A:212:LEU:HD12	2.02	0.41
1:A:276:PRO:HB2	1:A:300:LEU:HG	2.03	0.41
1:A:367:PHE:CE2	1:B:296:PHE:HB2	2.56	0.41
1:A:378:LEU:HD13	1:B:377:PHE:CE1	2.56	0.41
1:B:91:PHE:HE2	1:B:308:ALA:HB1	1.85	0.41
1:B:146:LEU:HD12	1:B:146:LEU:HA	1.89	0.41
1:B:177:GLY:HA3	1:B:280:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLY:O	1:B:423:PHE:HB3	2.19	0.41
2:G:229:LEU:O	2:G:233:LEU:HG	2.20	0.41
1:I:91:PHE:CB	1:I:417:ARG:HH22	2.34	0.41
1:J:40:SER:HB3	1:J:75:PHE:CD2	2.55	0.41
1:J:209:PHE:HA	1:J:212:LEU:HD12	2.03	0.41
1:J:286:PHE:CZ	1:J:393:LEU:HG	2.55	0.41
1:A:318:THR:HG22	1:A:322:ILE:HD11	2.02	0.41
1:B:130:VAL:HA	1:B:133:LEU:HG	2.02	0.41
2:G:22:VAL:HA	2:G:32:VAL:HG11	2.03	0.41
1:J:34:LEU:HD22	1:J:79:VAL:HG21	2.03	0.41
1:A:60:VAL:HB	1:A:176:ALA:HA	2.03	0.41
1:A:92:MET:HG3	1:A:133:LEU:HD22	2.02	0.41
1:A:319:PHE:CZ	1:A:323:LEU:HD22	2.56	0.41
1:A:377:PHE:CE1	1:B:378:LEU:HD13	2.56	0.41
1:A:434:ASN:OD1	1:A:435:ILE:HG23	2.21	0.41
1:B:129:LEU:HG	1:B:133:LEU:HD23	2.03	0.41
1:B:318:THR:HG22	1:B:322:ILE:HD11	2.02	0.41
1:B:390:THR:HG21	1:B:417:ARG:HB2	2.03	0.41
2:E:8:GLN:HB2	2:E:71:PHE:HA	2.03	0.41
2:G:218:VAL:HB	2:G:244:VAL:HG13	2.02	0.41
2:G:230:THR:O	2:G:234:LEU:HG	2.20	0.41
1:I:230:LEU:HD23	1:I:339:PHE:CE2	2.56	0.41
1:J:34:LEU:HB3	1:J:79:VAL:HG11	2.02	0.41
1:A:62:GLY:HA3	1:A:392:GLY:HA2	2.02	0.41
1:B:353:ALA:O	1:B:357:THR:OG1	2.21	0.41
2:D:63:LEU:HA	2:D:68:ILE:HD12	2.03	0.41
2:D:88:THR:O	2:D:92:LEU:HG	2.20	0.41
2:E:214:GLU:OE1	2:E:214:GLU:N	2.53	0.41
1:I:398:THR:HA	1:I:401:LEU:HG	2.03	0.40
1:A:69:GLY:HA3	1:A:180:LEU:O	2.20	0.40
1:A:227:HIS:HB2	1:B:442:VAL:HA	2.03	0.40
2:G:177:VAL:HA	2:G:195:VAL:O	2.21	0.40
1:J:318:THR:HG22	1:J:322:ILE:HD11	2.03	0.40
2:C:108:TYR:O	2:C:112:VAL:HG12	2.22	0.40
2:D:72:GLU:OE1	2:D:72:GLU:N	2.53	0.40
2:E:108:TYR:O	2:E:112:VAL:HG12	2.21	0.40
1:I:251:TYR:O	1:I:258:GLY:HA2	2.21	0.40
1:I:294:ILE:O	1:I:298:LEU:HD13	2.21	0.40
1:I:319:PHE:CZ	1:I:323:LEU:HD22	2.56	0.40
1:I:366:ILE:HD13	1:I:381:VAL:HG13	2.03	0.40
1:J:59:THR:O	1:J:60:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:322:ILE:HD11	1:J:351:ALA:O	2.21	0.40
2:C:12:ILE:HA	2:C:35:VAL:HG13	2.02	0.40
1:I:199:THR:HG21	1:I:270:TYR:HE2	1.86	0.40
1:J:270:TYR:O	1:J:274:VAL:HG23	2.21	0.40
1:J:361:ILE:HD13	1:J:415:ILE:HG21	2.03	0.40
1:A:250:GLU:OE2	1:A:293:THR:OG1	2.32	0.40
1:A:377:PHE:O	1:A:381:VAL:HG23	2.22	0.40
2:C:199:ALA:HB1	2:C:230:THR:HG23	2.02	0.40
2:D:16:ARG:NH1	2:D:247:GLN:O	2.55	0.40
2:E:85:SER:O	2:E:89:THR:HG23	2.21	0.40
2:E:175:LEU:HD21	2:E:208:LEU:HG	2.03	0.40
1:I:69:GLY:HA3	1:I:180:LEU:O	2.21	0.40
1:I:203:ILE:HD11	1:I:274:VAL:HG11	2.04	0.40
1:A:204:THR:O	1:A:212:LEU:HD21	2.21	0.40
1:A:244:LEU:O	1:A:248:ILE:HG12	2.21	0.40
1:B:436:ARG:HA	1:B:436:ARG:HD3	1.89	0.40
2:C:83:GLN:HE22	2:D:106:ASN:HD21	1.70	0.40
2:C:235:LYS:HA	2:C:235:LYS:HD2	1.90	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	402/445 (90%)	355 (88%)	43 (11%)	4 (1%)	15	54
1	B	402/445 (90%)	351 (87%)	47 (12%)	4 (1%)	15	54
1	I	402/445 (90%)	354 (88%)	47 (12%)	1 (0%)	47	81
1	J	402/445 (90%)	358 (89%)	41 (10%)	3 (1%)	22	62
2	C	264/288 (92%)	243 (92%)	21 (8%)	0	100	100
2	D	264/288 (92%)	246 (93%)	18 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	264/288 (92%)	244 (92%)	20 (8%)	0	100	100
2	G	264/288 (92%)	243 (92%)	21 (8%)	0	100	100
All	All	2664/2932 (91%)	2394 (90%)	258 (10%)	12 (0%)	29	69

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY
1	A	309	SER
1	B	258	GLY
1	J	310	THR
1	J	311	ALA
1	B	310	THR
1	J	309	SER
1	A	311	ALA
1	B	309	SER
1	I	332	GLY
1	A	332	GLY
1	B	332	GLY

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	335/374 (90%)	319 (95%)	16 (5%)	25	51
1	B	335/374 (90%)	322 (96%)	13 (4%)	32	56
1	I	335/374 (90%)	321 (96%)	14 (4%)	30	54
1	J	335/374 (90%)	319 (95%)	16 (5%)	25	51
2	C	222/240 (92%)	217 (98%)	5 (2%)	50	70
2	D	222/240 (92%)	221 (100%)	1 (0%)	88	93
2	E	222/240 (92%)	221 (100%)	1 (0%)	88	93
2	G	222/240 (92%)	217 (98%)	5 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2228/2456 (91%)	2157 (97%)	71 (3%)	39 61

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	34	LEU
1	I	60	VAL
1	I	63	LEU
1	I	73	THR
1	I	91	PHE
1	I	146	LEU
1	I	166	LEU
1	I	185	LEU
1	I	198	ILE
1	I	211	VAL
1	I	309	SER
1	I	310	THR
1	I	370	THR
1	I	421	LEU
1	J	34	LEU
1	J	48	ILE
1	J	60	VAL
1	J	73	THR
1	J	91	PHE
1	J	92	MET
1	J	137	SER
1	J	146	LEU
1	J	166	LEU
1	J	185	LEU
1	J	198	ILE
1	J	310	THR
1	J	352	LEU
1	J	370	THR
1	J	395	MET
1	J	421	LEU
1	A	34	LEU
1	A	48	ILE
1	A	63	LEU
1	A	66	VAL
1	A	73	THR
1	A	91	PHE
1	A	146	LEU

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Mol	Chain	Res	Type
1	A	166	LEU
1	A	185	LEU
1	A	198	ILE
1	A	211	VAL
1	A	257	LEU
1	A	272	GLN
1	A	310	THR
1	A	370	THR
1	A	421	LEU
1	B	34	LEU
1	B	63	LEU
1	B	66	VAL
1	B	73	THR
1	B	137	SER
1	B	146	LEU
1	B	166	LEU
1	B	185	LEU
1	B	198	ILE
1	B	211	VAL
1	B	310	THR
1	B	370	THR
1	B	421	LEU
2	C	28	MET
2	C	120	ARG
2	C	134	GLN
2	C	276	GLN
2	C	280	ASP
2	D	280	ASP
2	E	138	ASP
2	G	95	LEU
2	G	134	GLN
2	G	138	ASP
2	G	276	GLN
2	G	280	ASP

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

Mol	Chain	Res	Type
1	I	175	ASN
1	I	379	GLN
1	J	175	ASN
1	B	175	ASN

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Mol	Chain	Res	Type
2	C	83	GLN
2	G	203	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	406/445 (91%)	0.89	65 (16%)	1	4	356, 356, 356, 356	0
1	B	406/445 (91%)	0.88	61 (15%)	2	4	356, 356, 356, 356	0
1	I	406/445 (91%)	1.06	77 (18%)	1	3	357, 357, 357, 357	0
1	J	406/445 (91%)	0.91	61 (15%)	2	4	357, 357, 357, 357	0
2	C	268/288 (93%)	1.94	100 (37%)	0	1	371, 371, 371, 371	0
2	D	268/288 (93%)	2.48	145 (54%)	0	0	371, 371, 371, 371	0
2	E	268/288 (93%)	2.52	131 (48%)	0	1	371, 371, 371, 371	0
2	G	268/288 (93%)	2.00	107 (39%)	0	1	371, 371, 371, 371	0
All	All	2696/2932 (91%)	1.45	747 (27%)	0	2	356, 357, 371, 371	0

All (747) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	GLU	21.4
2	E	246	ALA	13.6
1	A	432	GLN	12.9
1	J	431	GLU	11.2
2	E	282	ASN	10.7
1	I	32	ALA	10.7
1	I	36	MET	10.1
2	E	56	ASN	9.9
2	E	245	LYS	9.7
2	E	103	LYS	9.5
2	E	247	GLN	9.4
2	C	95	LEU	9.3
1	A	430	THR	9.2
2	D	218	VAL	9.2
2	G	7	LYS	9.2
2	C	10	ALA	8.8

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Mol	Chain	Res	Type	RSRZ
2	E	259	GLY	8.8
2	C	7	LYS	8.6
1	J	259	HIS	8.5
2	G	176	ALA	8.4
2	E	57	ALA	8.4
2	E	77	ALA	8.3
2	D	200	THR	8.2
2	D	245	LYS	8.2
2	C	56	ASN	8.1
2	D	89	THR	8.1
2	G	282	ASN	8.1
2	E	176	ALA	8.0
2	E	55	ALA	8.0
2	D	58	THR	8.0
1	A	433	SER	7.9
2	E	264	ILE	7.9
1	B	71	GLN	7.8
2	C	118	ALA	7.7
2	D	244	VAL	7.7
2	D	11	VAL	7.6
2	D	251	HIS	7.6
2	D	153	VAL	7.6
2	C	96	ASP	7.6
2	D	140	ASN	7.4
2	G	153	VAL	7.4
2	E	194	ALA	7.3
2	D	255	LEU	7.3
2	D	154	ILE	7.3
1	B	284	LEU	7.3
2	C	152	ALA	7.3
2	G	152	ALA	7.2
2	E	76	VAL	7.2
2	C	93	LYS	7.2
1	A	370	THR	7.2
2	D	57	ALA	7.2
2	G	193	HIS	7.2
2	D	10	ALA	7.1
2	D	199	ALA	7.1
2	G	57	ALA	7.1
1	I	66	VAL	7.1
1	A	74	VAL	7.1
2	D	246	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
2	G	218	VAL	7.1
2	C	11	VAL	7.0
2	E	58	THR	6.9
1	I	50	ALA	6.9
2	E	11	VAL	6.9
2	E	35	VAL	6.9
2	D	227	SER	6.9
2	D	198	ASN	6.8
2	E	30	HIS	6.8
1	J	256	THR	6.8
2	C	117	GLY	6.7
2	D	250	TYR	6.7
1	A	158	TRP	6.7
2	E	281	GLU	6.7
2	E	260	ALA	6.7
2	E	265	HIS	6.7
2	D	220	ILE	6.7
2	E	50	THR	6.5
2	D	53	VAL	6.5
2	D	231	THR	6.5
1	A	38	PRO	6.4
2	G	9	PHE	6.4
2	G	13	GLY	6.4
2	G	58	THR	6.4
2	G	11	VAL	6.4
1	J	260	LEU	6.4
1	A	73	THR	6.4
2	E	94	GLU	6.3
2	C	57	ALA	6.3
2	G	35	VAL	6.3
1	B	42	THR	6.3
2	G	14	LEU	6.3
1	B	332	GLY	6.3
2	D	152	ALA	6.2
2	G	76	VAL	6.2
1	B	283	SER	6.2
1	I	437	TYR	6.2
2	C	55	ALA	6.1
2	G	151	PHE	6.1
2	E	95	LEU	6.0
2	D	55	ALA	6.0
2	G	194	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
2	E	195	VAL	5.9
2	D	263	ILE	5.9
2	E	29	GLY	5.9
2	E	13	GLY	5.8
1	I	35	LEU	5.8
2	E	51	HIS	5.8
2	G	34	ALA	5.8
2	D	282	ASN	5.8
1	J	257	LEU	5.8
2	G	30	HIS	5.8
2	E	244	VAL	5.7
2	E	255	LEU	5.7
1	B	190	GLY	5.7
2	E	280	ASP	5.7
2	G	199	ALA	5.7
1	B	195	ASN	5.7
2	C	9	PHE	5.6
1	B	45	LEU	5.6
2	D	63	LEU	5.6
1	A	39	ILE	5.6
1	J	284	LEU	5.6
2	G	77	ALA	5.6
2	D	73	TYR	5.6
2	E	140	ASN	5.6
2	C	31	GLU	5.5
1	A	159	SER	5.5
2	D	137	SER	5.5
2	G	175	LEU	5.5
2	E	263	ILE	5.5
2	G	31	GLU	5.5
1	A	75	PHE	5.5
1	I	151	ARG	5.5
2	E	218	VAL	5.5
2	G	29	GLY	5.5
2	C	258	ILE	5.4
2	E	53	VAL	5.4
2	E	258	ILE	5.4
2	E	34	ALA	5.4
2	D	253	LYS	5.3
2	G	192	THR	5.3
1	I	33	VAL	5.3
1	I	45	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	282	ASN	5.3
2	D	260	ALA	5.3
1	B	192	PRO	5.3
2	D	9	PHE	5.3
2	E	227	SER	5.3
1	I	37	LEU	5.2
1	B	193	THR	5.2
2	C	244	VAL	5.2
2	G	244	VAL	5.1
2	G	102	VAL	5.1
2	E	85	SER	5.1
1	B	285	ASP	5.1
1	B	331	ARG	5.1
2	C	210	ILE	5.1
1	J	151	ARG	5.1
1	B	164	ALA	5.1
2	D	90	LEU	5.1
2	E	14	LEU	5.0
2	G	154	ILE	5.0
2	G	60	GLU	5.0
2	C	263	ILE	5.0
1	B	333	LYS	5.0
2	G	281	GLU	5.0
2	E	104	ALA	5.0
1	J	255	GLY	5.0
2	E	251	HIS	5.0
2	D	60	GLU	5.0
1	I	47	TRP	5.0
2	E	102	VAL	5.0
2	C	94	GLU	4.9
2	D	136	LEU	4.9
1	J	262	ILE	4.9
2	C	8	GLN	4.9
2	C	89	THR	4.9
2	G	56	ASN	4.9
2	E	78	ILE	4.9
2	E	92	LEU	4.9
2	E	266	PRO	4.9
2	D	101	TRP	4.8
2	G	258	ILE	4.8
1	J	261	HIS	4.8
2	D	155	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	G	156	LEU	4.8
2	G	172	HIS	4.8
2	E	93	LYS	4.8
2	D	59	GLU	4.8
1	I	435	ILE	4.8
2	D	247	GLN	4.8
2	E	220	ILE	4.8
1	I	49	ASP	4.8
2	G	177	VAL	4.7
2	E	18	GLY	4.7
2	C	75	ILE	4.7
1	J	432	GLN	4.7
1	B	291	GLU	4.7
1	I	46	SER	4.7
1	I	44	PRO	4.7
2	C	30	HIS	4.7
1	J	336	THR	4.6
1	B	41	THR	4.6
2	D	177	VAL	4.6
2	E	175	LEU	4.6
1	B	254	PRO	4.6
1	A	403	THR	4.6
2	C	33	LEU	4.6
2	E	86	THR	4.6
1	B	152	LEU	4.6
2	E	231	THR	4.6
2	C	70	ASN	4.5
1	I	438	PRO	4.5
2	D	264	ILE	4.5
1	I	31	GLY	4.5
2	E	12	ILE	4.5
2	D	224	ILE	4.5
1	I	65	VAL	4.5
2	E	208	LEU	4.4
1	I	332	GLY	4.4
2	E	136	LEU	4.4
1	J	254	PRO	4.4
1	I	193	THR	4.4
2	D	230	THR	4.4
2	D	176	ALA	4.4
2	E	177	VAL	4.4
2	G	10	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	56	ASN	4.4
2	C	25	LEU	4.4
2	D	17	PHE	4.4
2	E	153	VAL	4.4
2	D	197	ALA	4.3
2	D	201	GLU	4.3
1	I	333	LYS	4.3
2	D	228	THR	4.3
2	G	217	ILE	4.3
2	D	234	LEU	4.3
1	A	36	MET	4.2
2	G	12	ILE	4.2
2	D	217	ILE	4.2
1	J	264	ASP	4.2
2	D	103	LYS	4.2
1	B	335	GLU	4.2
2	C	175	LEU	4.2
2	D	33	LEU	4.2
2	D	102	VAL	4.2
2	D	266	PRO	4.2
2	E	152	ALA	4.1
2	D	258	ILE	4.1
2	G	18	GLY	4.1
2	C	239	ILE	4.1
1	I	48	ILE	4.1
2	C	115	LYS	4.1
2	C	32	VAL	4.1
2	D	35	VAL	4.0
1	B	286	PHE	4.0
1	J	258	GLY	4.0
1	I	394	THR	4.0
2	C	34	ALA	4.0
1	B	255	GLY	4.0
2	G	59	GLU	4.0
2	C	218	VAL	4.0
2	D	249	TYR	4.0
2	D	76	VAL	4.0
2	E	224	ILE	4.0
2	G	200	THR	4.0
2	C	108	TYR	4.0
2	E	32	VAL	4.0
1	A	371	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	223	ASN	4.0
2	C	213	PHE	4.0
2	D	278	LEU	3.9
2	D	116	ILE	3.9
2	G	173	GLU	3.9
2	D	88	THR	3.9
2	D	254	VAL	3.9
2	E	215	TYR	3.9
2	G	191	ALA	3.9
1	A	375	ALA	3.9
1	B	191	ASP	3.9
1	I	152	LEU	3.9
2	G	245	LYS	3.9
2	D	281	GLU	3.9
2	E	96	ASP	3.9
2	E	234	LEU	3.9
1	B	72	PHE	3.9
2	G	85	SER	3.9
1	J	340	ARG	3.8
2	G	66	LEU	3.8
1	J	289	MET	3.8
2	G	227	SER	3.8
2	D	252	HIS	3.8
2	G	33	LEU	3.8
2	C	154	ILE	3.8
2	G	224	ILE	3.8
2	D	91	LEU	3.8
1	B	292	GLY	3.8
2	D	93	LYS	3.8
1	A	337	VAL	3.8
2	G	171	GLY	3.7
2	E	79	GLY	3.7
2	C	76	VAL	3.7
2	D	226	ALA	3.7
2	E	249	TYR	3.7
2	C	234	LEU	3.7
2	G	78	ILE	3.7
2	G	280	ASP	3.7
1	A	220	ARG	3.7
1	A	435	ILE	3.7
1	B	68	THR	3.7
2	E	154	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	G	75	ILE	3.7
1	I	436	ARG	3.7
2	D	118	ALA	3.7
2	C	264	ILE	3.7
1	A	368	ALA	3.7
2	C	113	LEU	3.7
2	D	7	LYS	3.7
2	C	116	ILE	3.7
2	D	115	LYS	3.7
2	D	78	ILE	3.7
2	G	210	ILE	3.7
2	D	248	ASN	3.6
2	D	18	GLY	3.6
2	G	55	ALA	3.6
2	C	73	TYR	3.6
2	D	34	ALA	3.6
2	D	119	ASP	3.6
2	E	219	ALA	3.6
1	J	293	THR	3.6
1	A	374	GLN	3.6
1	A	434	ASN	3.6
2	E	49	ALA	3.6
1	I	38	PRO	3.6
2	E	33	LEU	3.6
2	C	153	VAL	3.6
2	C	208	LEU	3.6
2	E	253	LYS	3.6
2	D	117	GLY	3.6
2	E	160	GLY	3.6
1	B	189	VAL	3.6
1	J	343	ILE	3.6
1	I	221	PHE	3.6
2	D	74	VAL	3.6
2	E	250	TYR	3.6
1	I	51	LEU	3.5
2	G	174	VAL	3.5
2	G	208	LEU	3.5
2	G	8	GLN	3.5
2	G	216	VAL	3.5
2	D	12	ILE	3.5
2	D	100	ILE	3.5
2	C	231	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	71	GLN	3.5
1	B	165	SER	3.5
2	C	255	LEU	3.5
2	D	219	ALA	3.5
2	E	216	VAL	3.5
1	B	70	THR	3.5
2	C	58	THR	3.5
2	D	204	GLU	3.5
2	E	22	VAL	3.5
1	B	43	LYS	3.5
2	D	151	PHE	3.5
2	C	194	ALA	3.5
2	E	59	GLU	3.5
2	E	193	HIS	3.5
2	C	216	VAL	3.5
1	J	149	SER	3.5
2	E	207	SER	3.5
1	J	148	LEU	3.5
2	C	69	ARG	3.5
1	I	178	PHE	3.5
2	D	54	ILE	3.4
2	C	119	ASP	3.4
2	D	61	ASN	3.4
1	A	37	LEU	3.4
2	E	196	ILE	3.4
1	J	250	GLU	3.4
2	G	155	GLY	3.4
1	A	424	VAL	3.4
2	D	92	LEU	3.4
1	A	340	ARG	3.4
2	E	54	ILE	3.4
1	J	152	LEU	3.4
1	J	246	VAL	3.4
2	D	259	GLY	3.4
2	C	67	GLY	3.4
1	J	245	THR	3.4
1	J	374	GLN	3.4
1	B	40	SER	3.4
2	C	111	LYS	3.3
1	J	430	THR	3.3
1	I	331	ARG	3.3
2	C	85	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	53	THR	3.3
2	E	91	LEU	3.3
1	J	285	ASP	3.3
2	G	116	ILE	3.3
1	J	192	PRO	3.3
2	C	74	VAL	3.3
2	G	53	VAL	3.3
1	I	30	ILE	3.3
1	A	426	SER	3.3
2	C	121	ILE	3.3
1	A	40	SER	3.3
1	B	288	SER	3.3
2	G	170	MET	3.3
2	C	66	LEU	3.3
2	G	220	ILE	3.2
1	B	67	ASP	3.2
2	D	75	ILE	3.2
2	D	66	LEU	3.2
2	G	279	SER	3.2
2	E	45	TYR	3.2
2	D	202	GLU	3.2
2	D	77	ALA	3.2
2	D	216	VAL	3.2
2	E	248	ASN	3.2
1	B	168	HIS	3.2
2	E	122	ILE	3.2
2	E	89	THR	3.2
2	E	278	LEU	3.2
1	B	35	LEU	3.2
2	D	233	LEU	3.1
2	D	104	ALA	3.1
2	E	159	PHE	3.1
2	C	211	ARG	3.1
1	I	64	ALA	3.1
2	D	14	LEU	3.1
2	D	64	LEU	3.1
1	B	77	GLN	3.1
2	E	269	ASP	3.1
2	C	86	THR	3.1
1	I	262	ILE	3.1
1	I	67	ASP	3.1
2	C	260	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	65	VAL	3.1
2	D	179	ILE	3.1
2	E	217	ILE	3.1
1	J	335	GLU	3.1
2	D	267	GLU	3.1
2	D	87	LEU	3.1
2	C	112	VAL	3.1
2	E	63	LEU	3.1
1	I	334	LYS	3.0
1	I	434	ASN	3.0
1	A	427	PHE	3.0
1	B	151	ARG	3.0
1	B	259	HIS	3.0
2	E	252	HIS	3.0
1	I	149	SER	3.0
1	J	281	PHE	3.0
2	G	36	ASP	3.0
1	J	193	THR	3.0
1	A	336	THR	3.0
2	D	86	THR	3.0
1	A	369	LEU	3.0
2	G	88	THR	3.0
1	B	149	SER	3.0
2	E	151	PHE	3.0
1	J	290	ARG	3.0
2	E	254	VAL	3.0
1	A	221	PHE	2.9
2	C	80	ALA	2.9
2	G	121	ILE	2.9
2	G	195	VAL	2.9
1	A	372	THR	2.9
2	E	257	LYS	2.9
1	J	376	PRO	2.9
1	J	265	LYS	2.9
2	D	30	HIS	2.9
2	E	223	ASN	2.9
2	G	63	LEU	2.9
1	B	15	THR	2.9
1	B	272	GLN	2.9
2	D	274	ILE	2.9
1	B	44	PRO	2.9
1	B	329	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	292	GLY	2.9
1	B	32	ALA	2.9
2	C	230	THR	2.9
2	G	164	VAL	2.9
1	A	436	ARG	2.9
1	I	197	VAL	2.9
2	C	237	LEU	2.9
2	D	121	ILE	2.9
2	G	198	ASN	2.9
1	B	267	TRP	2.8
2	E	52	ALA	2.8
2	D	95	LEU	2.8
2	D	262	ARG	2.8
2	D	265	HIS	2.8
2	G	278	LEU	2.8
2	G	73	TYR	2.8
2	E	210	ILE	2.8
2	D	205	LEU	2.8
2	D	243	TRP	2.8
2	E	28	MET	2.8
2	G	114	GLU	2.8
2	G	250	TYR	2.8
2	D	225	GLN	2.8
1	I	192	PRO	2.8
2	G	231	THR	2.8
1	J	195	ASN	2.8
2	C	137	SER	2.8
2	C	151	PHE	2.8
2	D	94	GLU	2.8
1	B	256	THR	2.8
2	C	223	ASN	2.8
1	J	190	GLY	2.8
2	C	235	LYS	2.8
1	J	49	ASP	2.8
2	C	217	ILE	2.8
2	D	232	LEU	2.8
2	E	36	ASP	2.8
2	E	68	ILE	2.8
2	D	222	ALA	2.8
2	D	52	ALA	2.7
1	J	337	VAL	2.7
2	D	133	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	230	THR	2.7
2	G	22	VAL	2.7
1	A	177	GLY	2.7
2	C	29	GLY	2.7
2	E	274	ILE	2.7
1	I	395	MET	2.7
2	G	122	ILE	2.7
1	B	334	LYS	2.7
2	E	277	SER	2.7
1	J	344	LYS	2.7
2	E	64	LEU	2.7
2	G	32	VAL	2.7
1	I	196	LEU	2.7
1	J	375	ALA	2.7
2	C	103	LYS	2.7
2	D	120	ARG	2.7
1	B	36	MET	2.7
2	D	99	ASN	2.7
2	D	42	VAL	2.7
1	J	44	PRO	2.7
2	G	62	GLU	2.7
1	I	34	LEU	2.7
2	G	21	ILE	2.6
1	J	66	VAL	2.6
1	B	432	GLN	2.6
1	J	433	SER	2.6
2	C	199	ALA	2.6
2	D	229	LEU	2.6
2	G	51	HIS	2.6
1	A	41	THR	2.6
1	A	157	GLY	2.6
2	C	209	GLY	2.6
2	G	17	PHE	2.6
2	G	230	THR	2.6
2	D	175	LEU	2.6
2	C	134	GLN	2.6
2	G	264	ILE	2.6
1	I	445	GLY	2.6
2	C	281	GLU	2.6
1	A	293	THR	2.6
2	G	228	THR	2.6
2	E	228	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	335	GLU	2.5
2	G	68	ILE	2.5
2	G	103	LYS	2.5
1	J	247	PHE	2.5
1	I	41	THR	2.5
2	D	195	VAL	2.5
2	C	238	ASP	2.5
1	A	437	TYR	2.5
1	I	313	GLY	2.5
2	E	48	TYR	2.5
2	G	92	LEU	2.5
1	A	338	ILE	2.5
2	D	32	VAL	2.5
2	E	190	TYR	2.5
2	D	62	GLU	2.5
2	D	190	TYR	2.5
2	C	42	VAL	2.5
2	D	65	SER	2.5
1	B	287	GLY	2.5
2	C	259	GLY	2.5
2	G	86	THR	2.5
2	G	219	ALA	2.5
1	I	291	GLU	2.5
2	G	89	THR	2.5
2	D	139	GLU	2.5
1	I	68	THR	2.5
1	A	428	ALA	2.5
2	C	222	ALA	2.5
2	G	15	GLY	2.4
2	C	92	LEU	2.4
2	G	255	LEU	2.4
1	I	304	GLY	2.4
1	A	423	PHE	2.4
2	E	17	PHE	2.4
2	E	191	ALA	2.4
1	I	210	THR	2.4
1	A	420	PRO	2.4
2	C	100	ILE	2.4
2	E	204	GLU	2.4
2	E	31	GLU	2.4
1	A	429	LYS	2.4
2	G	67	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	256	GLU	2.4
2	C	68	ILE	2.4
2	G	225	GLN	2.4
2	E	222	ALA	2.4
2	G	149	LYS	2.4
1	I	72	PHE	2.4
1	J	159	SER	2.4
1	A	62	GLY	2.4
2	D	178	ASP	2.4
1	J	272	GLN	2.4
1	A	367	PHE	2.4
2	C	195	VAL	2.4
2	C	228	THR	2.4
2	C	107	TYR	2.4
1	I	301	MET	2.4
1	B	66	VAL	2.4
1	I	398	THR	2.4
1	I	164	ALA	2.4
1	A	339	PHE	2.4
1	B	163	PHE	2.4
2	C	225	GLN	2.4
2	D	85	SER	2.4
2	D	164	VAL	2.4
2	D	242	ILE	2.4
2	D	122	ILE	2.4
2	E	242	ILE	2.4
1	I	148	LEU	2.4
2	E	270	MET	2.3
2	E	132	ILE	2.3
1	B	76	GLY	2.3
2	C	220	ILE	2.3
2	E	121	ILE	2.3
2	E	65	SER	2.3
2	E	137	SER	2.3
1	J	338	ILE	2.3
2	D	68	ILE	2.3
2	G	150	GLN	2.3
1	A	444	THR	2.3
1	A	66	VAL	2.3
2	D	172	HIS	2.3
2	D	80	ALA	2.3
1	A	341	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	247	PHE	2.3
1	A	394	THR	2.3
2	D	165	LYS	2.3
2	D	237	LEU	2.3
1	A	380	ILE	2.3
1	A	35	LEU	2.3
1	I	194	VAL	2.3
2	C	242	ILE	2.3
2	G	243	TRP	2.3
1	I	195	ASN	2.3
1	I	29	ILE	2.3
2	C	133	ALA	2.3
1	A	425	PHE	2.3
1	I	261	HIS	2.3
2	E	205	LEU	2.3
2	D	277	SER	2.3
2	C	88	THR	2.3
2	D	111	LYS	2.3
2	E	60	GLU	2.2
2	D	210	ILE	2.2
2	E	233	LEU	2.2
1	J	45	LEU	2.2
1	A	77	GLN	2.2
1	B	435	ILE	2.2
2	E	41	LYS	2.2
2	E	9	PHE	2.2
1	I	43	LYS	2.2
2	C	219	ALA	2.2
1	J	444	THR	2.2
2	C	104	ALA	2.2
1	I	222	LYS	2.2
1	I	384	THR	2.2
1	J	164	ALA	2.2
1	A	365	GLY	2.2
1	J	286	PHE	2.2
1	B	253	ASN	2.2
2	E	213	PHE	2.2
1	B	128	GLY	2.2
1	I	263	VAL	2.2
2	C	176	ALA	2.2
2	E	199	ALA	2.2
2	G	222	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	160	SER	2.2
1	A	277	ARG	2.2
2	E	47	SER	2.2
2	C	52	ALA	2.2
2	E	273	LYS	2.2
1	I	370	THR	2.2
1	J	429	LYS	2.2
2	D	51	HIS	2.2
1	B	264	ASP	2.2
1	I	225	SER	2.2
1	J	46	SER	2.2
1	A	76	GLY	2.2
1	A	404	ALA	2.2
1	B	295	VAL	2.2
2	C	77	ALA	2.2
2	E	174	VAL	2.1
1	I	303	ILE	2.1
1	A	33	VAL	2.1
1	I	350	LYS	2.1
1	A	269	SER	2.1
2	C	51	HIS	2.1
2	D	83	GLN	2.1
1	J	253	ASN	2.1
2	C	280	ASP	2.1
2	G	117	GLY	2.1
1	B	29	ILE	2.1
2	G	223	ASN	2.1
2	E	97	ILE	2.1
2	G	45	TYR	2.1
2	G	260	ALA	2.1
2	D	25	LEU	2.1
1	I	40	SER	2.1
1	A	160	SER	2.1
1	J	291	GLU	2.1
2	D	256	GLU	2.1
1	I	444	THR	2.1
2	D	108	TYR	2.1
1	I	15	THR	2.1
2	C	122	ILE	2.1
1	I	252	SER	2.1
1	I	399	PRO	2.1
2	D	279	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	336	THR	2.1
1	J	153	VAL	2.0
1	B	156	TYR	2.0
1	I	349	ILE	2.0
1	J	158	TRP	2.0
1	A	445	GLY	2.0
2	C	17	PHE	2.0
2	G	274	ILE	2.0
2	G	136	LEU	2.0
1	J	47	TRP	2.0
2	C	41	LYS	2.0
1	I	300	LEU	2.0
2	E	80	ALA	2.0
1	J	389	GLY	2.0
1	I	168	HIS	2.0
1	A	42	THR	2.0
2	E	124	PRO	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.