Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:46 am BST

PDB ID	:	6R7B
Title	:	Crystal structure of Csx1 in complex with cyclic oligoadenylate cOA4 conformation 1
Authors	:	Molina, R.; Montoya, G.; Sofos, N.; Stella, S.
Deposited on	:	2019-03-28
Resolution	:	3.12 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 following versions of software and data (see references ⓘ) were used in the production of this report:

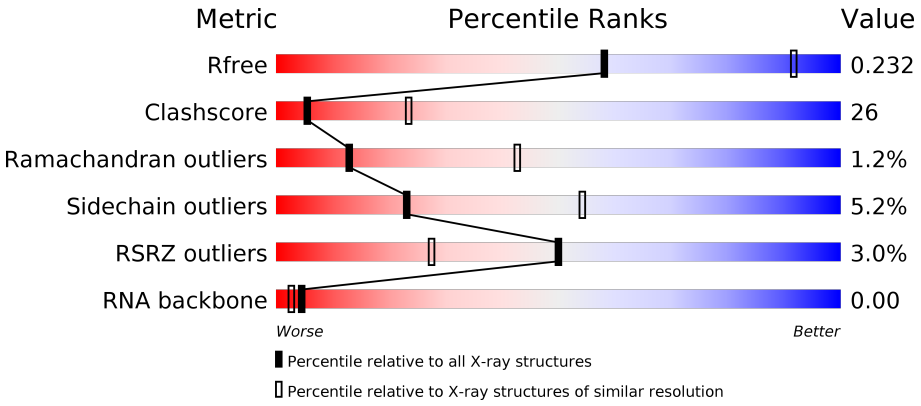
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.12 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	454	4% 60% 36% ·
1	B	454	5% 61% 35% ·
1	C	454	67% 31% ·
2	D	4	25% 75%

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Mol	Chain	Length	Quality of chain
2	E	4	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11153 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 CRISPR-associated (Cas) DxTHG family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			
1	B	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			
1	C	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			
2	E	2	Total	C	N	O	P	0	0	0
			44	20	10	12	2			

- Molecule 3 is water.

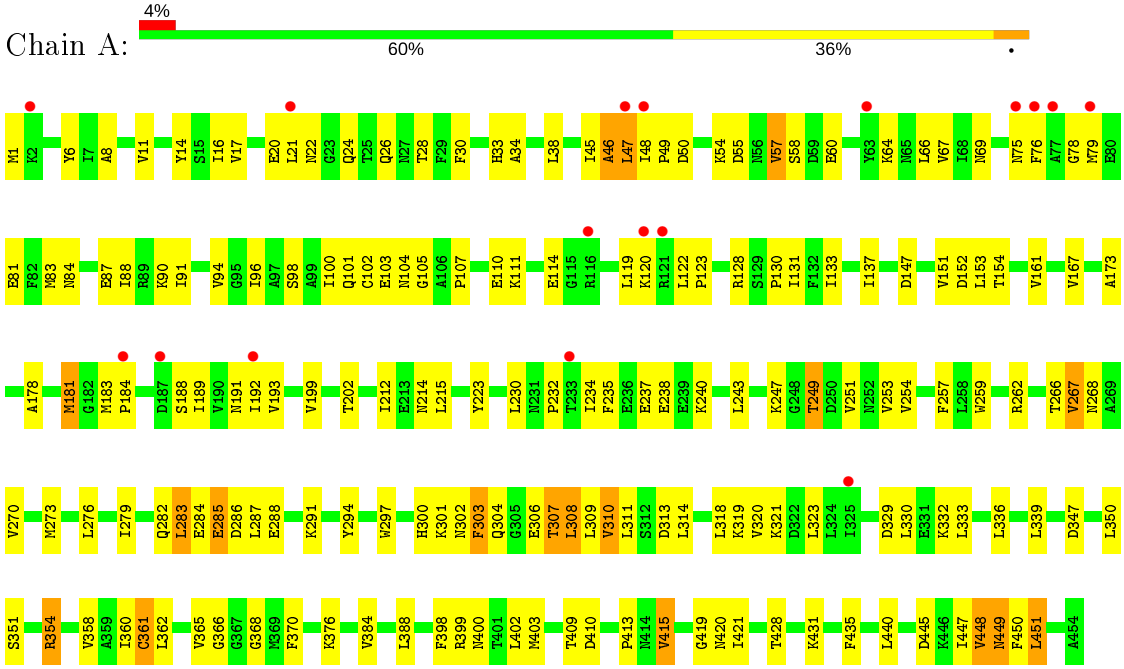
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	29	Total	O	0	0
			29	29		
3	C	45	Total	O	0	0
			45	45		

3 Residue-property plots (i)

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

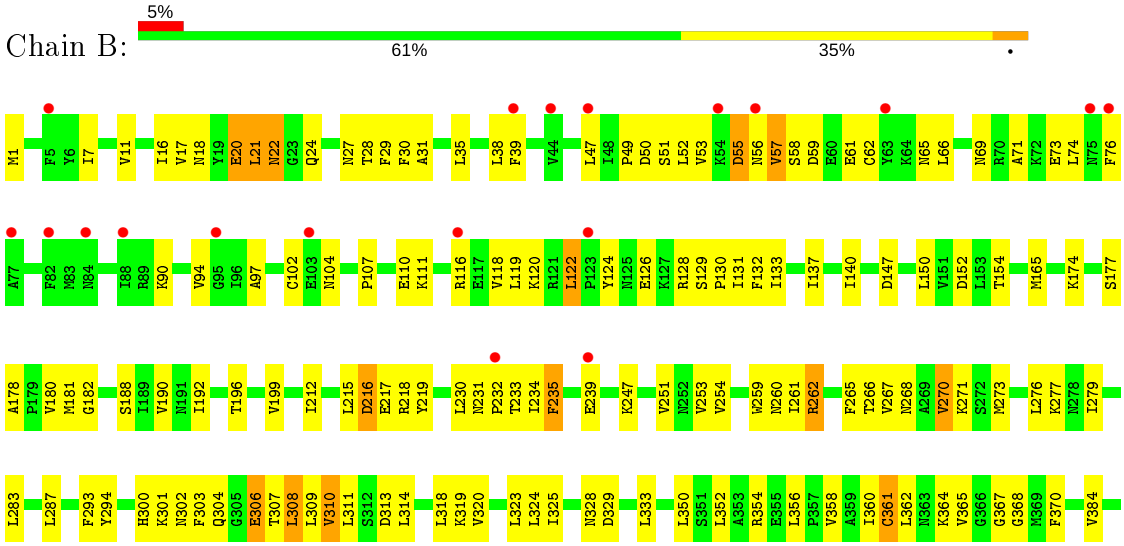
- Molecule 1: CRISPR-associated (Cas) DxTHG family

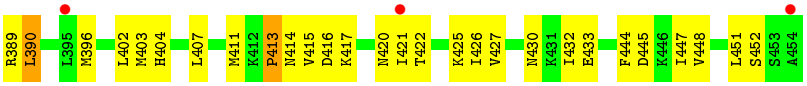
Chain A:



- Molecule 1: CRISPR-associated (Cas) DxTHG family

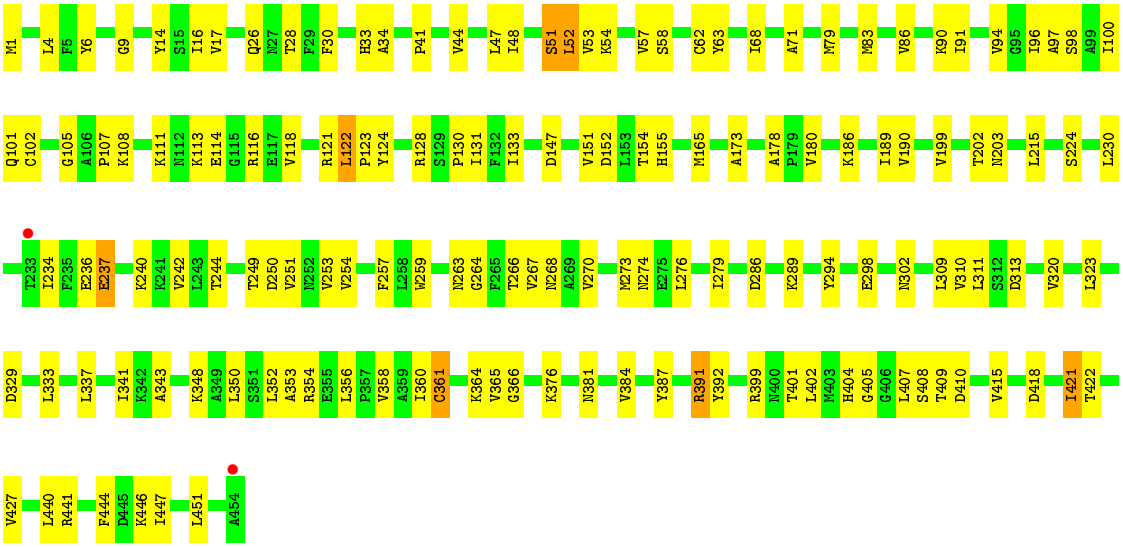
Chain B:





• Molecule 1: CRISPR-associated (Cas) DxTHG family

Chain C:



• Molecule 2: RNA (5'-R(P*AP*AP*AP*A)-3')

Chain D:

• Molecule 2: RNA (5'-R(P*AP*AP*AP*A)-3')

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.08Å 117.68Å 357.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 3.12 48.29 – 3.12	Depositor EDS
% Data completeness (in resolution range)	60.3 (48.29-3.12) 60.2 (48.29-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.180 , 0.229 0.225 , 0.232	Depositor DCC
R_{free} test set	1180 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	107.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 108.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11153	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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	0.52	0/3703	0.79	0/4990
1	B	0.52	0/3703	0.77	0/4990
1	C	0.53	0/3703	0.78	0/4990
2	D	0.93	0/99	0.92	0/152
2	E	0.99	0/49	1.16	0/74
All	All	0.53	0/11257	0.79	0/15196

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	3642	0	3675	258	0
1	B	3642	0	3675	205	0
1	C	3642	0	3675	140	0
2	D	88	0	44	6	0
2	E	44	0	23	6	0
3	A	21	0	0	0	0
3	B	29	0	0	0	0
3	C	45	0	0	1	0
All	All	11153	0	11092	573	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 26.

All (573) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:CG1	1:C:96:ILE:CD1	1.75	1.58
1:A:181:MET:HG3	2:D:1:A:C2	1.64	1.33
1:A:33:HIS:CE1	1:A:79:MET:CE	2.26	1.17
1:A:266:THR:HG22	1:A:336:LEU:CD2	1.74	1.16
1:A:17:VAL:HG12	1:A:188:SER:HB3	1.30	1.12
1:A:33:HIS:CE1	1:A:79:MET:HE1	1.85	1.10
1:A:266:THR:HG22	1:A:336:LEU:HD21	1.28	1.09
1:A:47:LEU:HD12	1:A:48:ILE:HG13	1.17	1.08
1:B:57:VAL:HG23	1:B:58:SER:H	1.09	1.07
1:C:387:TYR:CE1	1:C:391:ARG:HG2	1.90	1.07
1:A:310:VAL:CG1	1:A:313:ASP:HB2	1.86	1.04
1:B:267:VAL:HG23	1:B:268:ASN:HD22	1.22	1.04
1:C:356:LEU:HD23	1:C:444:PHE:HZ	1.22	1.04
1:A:287:LEU:HD13	1:A:318:LEU:HD11	1.39	1.04
1:C:356:LEU:HD23	1:C:444:PHE:CZ	1.94	1.01
1:A:232:PRO:HG2	1:A:235:PHE:CD2	1.95	1.00
1:A:103:GLU:HG2	1:A:104:ASN:H	1.22	1.00
1:B:73:GLU:O	1:B:74:LEU:HG	1.63	0.99
1:A:47:LEU:CD1	1:A:48:ILE:HG13	1.93	0.98
1:A:235:PHE:CE1	1:A:240:LYS:HG3	1.99	0.96
1:A:16:ILE:HD12	1:A:76:PHE:HZ	1.28	0.96
1:B:356:LEU:HD23	1:B:444:PHE:HZ	1.31	0.95
1:B:21:LEU:HB2	1:B:192:ILE:HG13	1.44	0.95
1:C:259:TRP:CE2	1:C:263:ASN:ND2	2.34	0.95
1:B:356:LEU:HD23	1:B:444:PHE:CZ	2.03	0.94
1:B:180:VAL:HG13	1:B:190:VAL:HG21	1.51	0.92
1:A:110:GLU:HB2	1:A:119:LEU:HB2	1.52	0.91
1:A:57:VAL:HG12	1:A:58:SER:H	1.35	0.90
1:A:33:HIS:HE1	1:A:79:MET:CE	1.74	0.89
1:A:276:LEU:HD23	1:A:279:ILE:HD12	1.53	0.89
1:B:426:ILE:HG13	1:B:427:VAL:H	1.37	0.89
1:A:365:VAL:HG12	1:A:376:LYS:HD3	1.53	0.88
1:A:235:PHE:HE1	1:A:240:LYS:HG3	1.34	0.88
1:B:57:VAL:HG23	1:B:58:SER:N	1.87	0.88
1:C:111:LYS:HG2	1:C:116:ARG:HA	1.55	0.88
1:B:358:VAL:HG22	1:B:384:VAL:HG21	1.53	0.88
1:B:267:VAL:HG23	1:B:268:ASN:ND2	1.89	0.88
1:A:75:ASN:O	1:A:76:PHE:CD1	2.27	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HD23	1:C:279:ILE:HD12	1.53	0.87
1:C:71:ALA:HB2	1:C:79:MET:HG3	1.54	0.87
1:A:310:VAL:HG12	1:A:313:ASP:HB2	1.56	0.86
1:A:398:PHE:HD2	1:A:435:PHE:CD2	1.94	0.86
1:A:310:VAL:HG11	1:A:313:ASP:CG	1.95	0.86
1:A:266:THR:HG22	1:A:336:LEU:HD23	1.56	0.85
1:C:111:LYS:HE2	1:C:116:ARG:HB2	1.57	0.85
1:A:16:ILE:HD12	1:A:76:PHE:CZ	2.12	0.85
1:A:287:LEU:CD2	1:A:291:LYS:HE2	2.07	0.85
1:A:21:LEU:O	1:A:22:ASN:OD1	1.96	0.84
1:C:354:ARG:HH22	1:C:381:ASN:HD21	1.24	0.84
1:B:21:LEU:HD12	1:B:38:LEU:HD11	1.57	0.84
1:A:301:LYS:O	1:A:304:GLN:HB2	1.77	0.84
1:A:310:VAL:HG11	1:A:313:ASP:HB2	1.58	0.84
1:B:364:LYS:HE3	1:B:452:SER:HA	1.60	0.83
1:C:52:LEU:O	1:C:52:LEU:HD12	1.75	0.83
1:B:180:VAL:CG1	1:B:190:VAL:HG21	2.08	0.83
1:A:310:VAL:HG11	1:A:313:ASP:CB	2.09	0.83
1:A:232:PRO:HG2	1:A:235:PHE:CE2	2.14	0.82
1:A:103:GLU:HG2	1:A:104:ASN:N	1.95	0.81
1:A:57:VAL:HG12	1:A:58:SER:N	1.96	0.81
1:A:181:MET:HG3	2:D:1:A:N1	1.95	0.81
1:B:21:LEU:HB2	1:B:192:ILE:CG1	2.09	0.81
1:A:24:GLN:H	1:A:24:GLN:NE2	1.78	0.80
1:A:235:PHE:HE1	1:A:240:LYS:CG	1.94	0.80
1:C:387:TYR:O	1:C:391:ARG:HB2	1.82	0.80
1:B:390:LEU:O	1:B:390:LEU:HD12	1.80	0.80
1:B:310:VAL:HG12	1:B:313:ASP:HB2	1.64	0.79
1:A:75:ASN:OD1	1:A:75:ASN:O	2.00	0.79
1:A:33:HIS:CE1	1:A:79:MET:SD	2.76	0.79
1:A:307:THR:HA	1:B:131:ILE:HG12	1.64	0.78
1:B:55:ASP:HB3	1:B:102:CYS:HB2	1.65	0.77
1:A:33:HIS:HE1	1:A:79:MET:HE1	1.30	0.77
1:B:253:VAL:HG12	1:B:276:LEU:HD11	1.66	0.76
1:C:407:LEU:HD23	1:C:407:LEU:N	2.00	0.76
1:A:33:HIS:ND1	1:A:79:MET:SD	2.59	0.76
1:A:249:THR:OG1	1:A:283:LEU:HD11	1.85	0.76
1:A:287:LEU:HD23	1:A:291:LYS:HE2	1.68	0.76
1:A:361:CYS:HB2	1:A:451:LEU:HD21	1.68	0.76
1:C:259:TRP:CZ2	1:C:263:ASN:ND2	2.54	0.75
1:A:47:LEU:HD12	1:A:48:ILE:CG1	2.09	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:HB2	1:B:116:ARG:HG2	1.68	0.75
1:B:174:LYS:HA	1:B:196:THR:HG22	1.67	0.75
1:A:287:LEU:HD13	1:A:318:LEU:CD1	2.16	0.75
1:B:356:LEU:HG	1:B:360:ILE:CD1	2.16	0.75
1:A:45:ILE:HD12	1:A:45:ILE:N	2.02	0.75
1:B:217:GLU:OE1	1:B:262:ARG:HB3	1.87	0.74
1:A:66:LEU:HD12	1:A:67:VAL:N	2.02	0.74
1:A:96:ILE:HG13	1:B:180:VAL:HG12	1.68	0.74
1:C:354:ARG:HG2	1:C:399:ARG:CZ	2.18	0.74
1:B:69:ASN:ND2	1:B:107:PRO:HD2	2.03	0.73
1:A:310:VAL:CG1	1:A:313:ASP:CB	2.63	0.73
1:B:426:ILE:HG13	1:B:427:VAL:N	2.03	0.72
1:B:57:VAL:CG2	1:B:58:SER:H	1.90	0.72
1:A:235:PHE:HE1	1:A:240:LYS:CB	2.03	0.72
1:A:64:LYS:HE2	1:A:84:ASN:HA	1.72	0.72
1:B:154:THR:OG1	1:B:177:SER:HA	1.90	0.72
1:B:28:THR:HG22	1:B:76:PHE:CZ	2.25	0.71
1:A:282:GLN:O	1:A:285:GLU:HG3	1.91	0.71
1:C:415:VAL:HG22	1:C:421:ILE:HD13	1.72	0.71
1:A:33:HIS:CE1	1:A:79:MET:HE2	2.21	0.71
1:A:64:LYS:CE	1:A:84:ASN:HA	2.21	0.70
1:B:21:LEU:HD13	1:B:21:LEU:O	1.90	0.70
1:C:350:LEU:HD23	1:C:440:LEU:HD13	1.72	0.70
1:A:267:VAL:HG23	1:A:268:ASN:H	1.56	0.70
1:A:154:THR:CG2	1:A:178:ALA:HB3	2.22	0.69
1:C:121:ARG:C	1:C:123:PRO:HD3	2.12	0.69
1:B:17:VAL:HG23	1:B:188:SER:HB2	1.74	0.69
1:C:51:SER:HB2	1:C:124:TYR:CD2	2.27	0.69
1:C:415:VAL:HG22	1:C:421:ILE:HG23	1.74	0.69
1:A:388:LEU:HD11	1:A:447:ILE:HD13	1.74	0.69
1:A:287:LEU:CD2	1:A:291:LYS:CE	2.71	0.69
1:A:350:LEU:HD12	1:A:402:LEU:HD12	1.73	0.69
1:A:360:ILE:HD13	1:A:448:VAL:HG22	1.73	0.69
1:A:330:LEU:HD13	1:B:421:ILE:HD11	1.74	0.68
1:A:398:PHE:CD2	1:A:435:PHE:CD2	2.80	0.68
1:C:51:SER:HB2	1:C:124:TYR:CG	2.29	0.68
1:B:51:SER:HB3	1:B:124:TYR:CE1	2.29	0.68
1:A:154:THR:HG21	1:A:178:ALA:HB3	1.75	0.68
1:A:287:LEU:HD23	1:A:291:LYS:CE	2.23	0.68
1:A:360:ILE:HD13	1:A:448:VAL:CG2	2.22	0.68
1:B:110:GLU:HB2	1:B:119:LEU:HD22	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PHE:CE1	1:A:240:LYS:CG	2.74	0.68
1:B:266:THR:HB	1:B:333:LEU:CD2	2.23	0.68
1:A:266:THR:CG2	1:A:336:LEU:HD23	2.23	0.68
1:B:310:VAL:CG1	1:B:313:ASP:H	2.06	0.68
1:C:52:LEU:O	1:C:100:ILE:HD12	1.93	0.68
1:A:419:GLY:O	1:B:328:ASN:HB2	1.93	0.68
1:C:230:LEU:O	1:C:230:LEU:HD23	1.94	0.68
1:A:75:ASN:O	1:A:76:PHE:HD1	1.72	0.68
1:B:415:VAL:HG23	1:B:421:ILE:HD12	1.76	0.68
1:A:368:GLY:O	1:B:415:VAL:HG12	1.93	0.67
1:B:69:ASN:HD21	1:B:107:PRO:HD2	1.57	0.67
1:C:259:TRP:CD2	1:C:263:ASN:ND2	2.61	0.67
1:C:113:LYS:HG2	1:C:114:GLU:HG3	1.75	0.67
1:A:249:THR:CG2	1:A:283:LEU:HD11	2.24	0.67
1:B:310:VAL:HG12	1:B:313:ASP:CB	2.23	0.67
1:C:111:LYS:HG2	1:C:116:ARG:CA	2.25	0.67
1:B:174:LYS:HA	1:B:196:THR:CG2	2.24	0.67
1:A:234:ILE:HD12	1:A:234:ILE:O	1.94	0.66
1:C:356:LEU:HG	1:C:360:ILE:CD1	2.26	0.66
1:A:120:LYS:HA	1:A:122:LEU:HD13	1.76	0.66
1:B:293:PHE:HB3	1:B:300:HIS:CD2	2.30	0.66
1:C:387:TYR:CE1	1:C:391:ARG:CG	2.76	0.66
1:A:102:CYS:HA	1:A:107:PRO:HA	1.78	0.65
1:C:71:ALA:CB	1:C:79:MET:HG3	2.25	0.65
1:A:303:PHE:HA	1:A:306:GLU:CG	2.27	0.65
1:B:356:LEU:HG	1:B:360:ILE:HD12	1.79	0.65
1:B:53:VAL:CG2	1:B:102:CYS:SG	2.85	0.65
1:A:235:PHE:CE1	1:A:240:LYS:HA	2.31	0.64
1:B:55:ASP:N	1:B:59:ASP:OD1	2.25	0.64
1:A:28:THR:HG21	1:A:33:HIS:ND1	2.12	0.64
1:C:408:SER:OG	1:C:410:ASP:HB2	1.98	0.64
1:B:51:SER:HB3	1:B:124:TYR:CZ	2.33	0.64
1:A:137:ILE:HG22	1:A:167:VAL:HG11	1.78	0.64
1:B:310:VAL:HG12	1:B:313:ASP:H	1.62	0.64
1:A:306:GLU:O	1:B:131:ILE:HD11	1.98	0.64
1:A:365:VAL:HG11	1:A:376:LYS:HG2	1.80	0.64
1:B:390:LEU:C	1:B:390:LEU:HD12	2.18	0.63
1:A:276:LEU:HD23	1:A:279:ILE:CD1	2.26	0.63
1:C:266:THR:HG21	1:C:352:LEU:HD13	1.80	0.63
1:A:131:ILE:HD13	1:B:307:THR:HA	1.80	0.63
1:B:69:ASN:ND2	1:B:107:PRO:CD	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:HG3	1:A:111:LYS:O	1.98	0.63
1:A:285:GLU:O	1:A:288:GLU:N	2.31	0.63
1:A:310:VAL:HG11	1:A:313:ASP:OD2	1.98	0.63
1:A:358:VAL:HG22	1:A:384:VAL:HG21	1.81	0.63
1:C:267:VAL:HG13	1:C:268:ASN:H	1.64	0.63
1:B:303:PHE:HA	1:B:306:GLU:HG2	1.79	0.63
1:C:350:LEU:HD12	1:C:402:LEU:HD12	1.79	0.63
1:A:98:SER:CA	1:A:122:LEU:HB3	2.30	0.62
1:B:310:VAL:HG11	1:B:313:ASP:CG	2.20	0.62
1:C:154:THR:CG2	1:C:178:ALA:HB3	2.29	0.62
1:C:52:LEU:C	1:C:52:LEU:HD12	2.18	0.62
1:B:356:LEU:HG	1:B:360:ILE:HD11	1.80	0.62
1:C:415:VAL:CG2	1:C:421:ILE:HG23	2.30	0.62
1:C:68:ILE:HD13	1:C:79:MET:HB3	1.82	0.62
1:A:14:TYR:HA	2:D:4:A:N7	2.15	0.61
1:B:27:ASN:O	1:B:28:THR:HG23	2.00	0.61
1:A:351:SER:HA	1:A:399:ARG:HE	1.65	0.61
1:A:365:VAL:CG1	1:A:376:LYS:HD3	2.27	0.61
1:A:413:PRO:HD2	1:B:370:PHE:HB2	1.82	0.61
1:B:38:LEU:HD22	1:B:39:PHE:CE2	2.35	0.61
1:A:8:ALA:HB3	1:A:48:ILE:HG23	1.83	0.61
1:B:154:THR:CG2	1:B:178:ALA:O	2.48	0.61
1:C:131:ILE:HD12	1:C:131:ILE:H	1.66	0.61
1:A:55:ASP:HB2	1:A:103:GLU:O	2.00	0.61
1:A:270:VAL:HG13	1:A:332:LYS:HB3	1.81	0.61
1:A:235:PHE:CE1	1:A:240:LYS:CB	2.83	0.61
1:C:407:LEU:HD23	1:C:407:LEU:H	1.66	0.61
1:C:415:VAL:HG22	1:C:421:ILE:CG2	2.30	0.61
1:C:44:VAL:HG12	1:C:86:VAL:HG23	1.81	0.61
1:A:267:VAL:HG23	1:A:268:ASN:N	2.15	0.61
1:A:309:LEU:O	1:B:131:ILE:HD13	2.01	0.61
1:C:337:LEU:HD23	1:C:441:ARG:HH11	1.65	0.61
1:A:361:CYS:HB2	1:A:451:LEU:CD2	2.31	0.61
1:B:21:LEU:C	1:B:21:LEU:HD13	2.20	0.61
1:C:392:TYR:OH	1:C:446:LYS:HD3	1.99	0.61
1:B:137:ILE:O	1:B:140:ILE:HG13	2.01	0.60
1:B:260:ASN:O	1:B:265:PHE:N	2.30	0.60
1:C:365:VAL:O	1:C:365:VAL:HG23	2.01	0.60
1:C:427:VAL:O	1:C:427:VAL:HG23	2.01	0.60
1:C:350:LEU:CD2	1:C:440:LEU:HD13	2.32	0.60
1:C:154:THR:HG21	1:C:178:ALA:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:O	1:B:74:LEU:HD12	2.01	0.60
1:A:276:LEU:HA	1:A:279:ILE:HD12	1.84	0.60
1:B:217:GLU:CD	1:B:262:ARG:NE	2.55	0.60
1:B:320:VAL:HG23	1:B:323:LEU:HD12	1.82	0.60
1:B:232:PRO:HG2	1:B:306:GLU:OE2	2.02	0.59
1:B:276:LEU:HA	1:B:279:ILE:HD12	1.84	0.59
1:A:347:ASP:N	1:A:402:LEU:HD13	2.18	0.59
1:A:45:ILE:H	1:A:45:ILE:HD12	1.65	0.59
1:A:249:THR:OG1	1:A:283:LEU:CD1	2.49	0.59
1:A:249:THR:HG21	1:A:283:LEU:HD11	1.85	0.59
1:B:53:VAL:HG22	1:B:102:CYS:SG	2.42	0.59
1:A:270:VAL:HG21	1:A:333:LEU:CD2	2.32	0.59
1:C:251:VAL:O	1:C:254:VAL:HG12	2.03	0.59
1:A:304:GLN:NE2	1:B:126:GLU:OE2	2.36	0.59
1:A:307:THR:HA	1:B:131:ILE:CG1	2.32	0.59
1:B:287:LEU:HD22	1:B:318:LEU:HD11	1.85	0.59
1:B:31:ALA:HB3	1:B:152:ASP:OD2	2.02	0.59
1:A:235:PHE:HE1	1:A:240:LYS:HA	1.68	0.58
1:A:285:GLU:O	1:A:288:GLU:CB	2.51	0.58
1:C:276:LEU:HA	1:C:279:ILE:HD12	1.85	0.58
1:C:310:VAL:HG12	1:C:313:ASP:H	1.68	0.58
1:C:48:ILE:HD12	1:C:63:TYR:HB2	1.84	0.58
1:A:114:GLU:N	1:A:114:GLU:OE1	2.37	0.58
1:A:131:ILE:H	1:A:131:ILE:HD12	1.67	0.58
1:B:218:ARG:HG2	1:B:218:ARG:O	2.03	0.58
1:B:232:PRO:O	1:B:235:PHE:CD1	2.56	0.58
1:C:111:LYS:CG	1:C:116:ARG:HA	2.32	0.58
1:C:276:LEU:HD23	1:C:279:ILE:CD1	2.27	0.58
1:A:283:LEU:HA	1:A:286:ASP:OD1	2.04	0.58
1:B:365:VAL:O	1:B:365:VAL:HG22	2.04	0.58
1:B:217:GLU:OE2	1:B:262:ARG:HD2	2.03	0.58
1:B:414:ASN:O	1:B:415:VAL:HG12	2.04	0.58
1:B:7:ILE:HG12	1:B:47:LEU:HD22	1.86	0.58
1:C:257:PHE:HB2	1:C:276:LEU:HD11	1.85	0.57
1:B:230:LEU:HB3	1:B:247:LYS:HG3	1.85	0.57
1:B:301:LYS:HG3	1:B:304:GLN:HB3	1.86	0.57
1:A:17:VAL:HG12	1:A:188:SER:CB	2.19	0.57
1:A:310:VAL:O	1:A:314:LEU:HD13	2.04	0.57
1:A:266:THR:CG2	1:A:336:LEU:CD2	2.65	0.57
1:C:358:VAL:HG22	1:C:384:VAL:HG21	1.86	0.57
1:A:17:VAL:CG1	1:A:184:PRO:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG12	1:A:376:LYS:CD	2.31	0.57
1:C:230:LEU:HD11	1:C:309:LEU:HB2	1.86	0.57
1:A:303:PHE:O	1:B:132:PHE:CD1	2.58	0.57
1:B:266:THR:HG21	1:B:352:LEU:HD13	1.86	0.57
1:A:251:VAL:O	1:A:254:VAL:HG12	2.04	0.57
1:A:96:ILE:CG1	1:B:180:VAL:HG12	2.35	0.57
1:C:234:ILE:CG2	1:C:302:ASN:HD22	2.17	0.57
1:A:320:VAL:HG23	1:A:323:LEU:HD12	1.87	0.57
1:B:251:VAL:O	1:B:254:VAL:HG12	2.05	0.57
1:A:415:VAL:HB	1:A:421:ILE:HG12	1.87	0.56
1:B:16:ILE:HD13	1:B:29:PHE:HB3	1.87	0.56
1:C:57:VAL:HG13	1:C:58:SER:H	1.70	0.56
1:A:266:THR:HB	1:A:333:LEU:CD2	2.35	0.56
1:B:51:SER:CB	1:B:124:TYR:CE1	2.88	0.56
1:B:31:ALA:CB	1:B:152:ASP:OD2	2.54	0.56
1:B:217:GLU:HG3	1:B:259:TRP:HD1	1.71	0.56
1:C:356:LEU:CD2	1:C:444:PHE:HZ	2.09	0.56
1:A:370:PHE:HD2	1:B:413:PRO:O	1.89	0.56
1:B:215:LEU:HD22	1:B:261:ILE:HG21	1.88	0.56
1:C:356:LEU:HG	1:C:360:ILE:HD12	1.87	0.56
1:C:387:TYR:CZ	1:C:391:ARG:CG	2.89	0.56
1:A:366:GLY:HA2	1:B:417:LYS:HG3	1.88	0.56
1:A:257:PHE:HB2	1:A:276:LEU:HD11	1.88	0.55
1:A:300:HIS:HB3	1:A:303:PHE:HE2	1.71	0.55
1:B:18:ASN:CB	1:B:27:ASN:HB3	2.36	0.55
1:C:253:VAL:HG12	1:C:276:LEU:HD21	1.87	0.55
1:A:54:LYS:O	1:A:54:LYS:HG3	2.06	0.55
1:A:421:ILE:O	1:B:271:LYS:HE2	2.06	0.55
1:B:97:ALA:O	1:B:122:LEU:HD23	2.06	0.55
1:C:267:VAL:HG13	1:C:268:ASN:N	2.20	0.55
1:A:69:ASN:O	1:A:69:ASN:OD1	2.25	0.55
1:B:111:LYS:HD2	1:B:116:ARG:HG2	1.87	0.55
1:B:310:VAL:HG12	1:B:310:VAL:O	2.06	0.55
1:A:235:PHE:HE1	1:A:240:LYS:CA	2.20	0.55
1:A:50:ASP:HA	1:A:90:LYS:HE2	1.89	0.55
1:B:119:LEU:HD12	1:B:120:LYS:H	1.72	0.55
1:B:303:PHE:HA	1:B:306:GLU:CG	2.36	0.55
1:B:38:LEU:HD22	1:B:39:PHE:CZ	2.42	0.55
1:B:69:ASN:HD22	1:B:107:PRO:CG	2.20	0.55
1:A:212:ILE:HD13	1:A:319:LYS:HB3	1.89	0.55
1:A:21:LEU:HD22	1:A:38:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:HG2	1:A:34:ALA:HA	1.88	0.55
1:B:407:LEU:N	1:B:407:LEU:HD12	2.22	0.55
1:A:303:PHE:HA	1:A:306:GLU:HG2	1.89	0.54
1:A:415:VAL:HA	1:A:420:ASN:O	2.07	0.54
1:B:51:SER:OG	1:B:51:SER:O	2.24	0.54
2:E:2:A:H2'	2:E:2:A:N3	2.21	0.54
1:A:370:PHE:CD2	1:B:413:PRO:O	2.60	0.54
1:B:154:THR:HG23	1:B:178:ALA:O	2.06	0.54
1:B:362:LEU:O	1:B:367:GLY:N	2.40	0.54
1:A:330:LEU:CD1	1:B:421:ILE:HD11	2.36	0.54
1:C:94:VAL:HG13	1:C:128:ARG:H	1.72	0.54
1:B:212:ILE:HD13	1:B:319:LYS:HB3	1.89	0.54
1:A:192:ILE:CG2	1:A:193:VAL:N	2.70	0.54
1:B:50:ASP:HA	1:B:90:LYS:HE2	1.90	0.54
1:C:48:ILE:HD11	1:C:53:VAL:HG12	1.88	0.54
1:A:270:VAL:HG21	1:A:333:LEU:HD23	1.90	0.54
1:C:53:VAL:CG2	1:C:102:CYS:SG	2.96	0.54
1:C:6:TYR:CB	1:C:152:ASP:HB3	2.38	0.53
1:C:350:LEU:HD23	1:C:440:LEU:CD1	2.38	0.53
1:B:310:VAL:CG1	1:B:313:ASP:CG	2.77	0.53
1:C:48:ILE:HG23	1:C:90:LYS:HA	1.89	0.53
1:B:18:ASN:HB3	1:B:27:ASN:HB3	1.89	0.53
1:A:8:ALA:HB3	1:A:48:ILE:CG2	2.38	0.53
1:A:6:TYR:CB	1:A:152:ASP:HB3	2.39	0.53
1:C:101:GLN:HG3	1:C:108:LYS:HD3	1.91	0.53
1:C:165:MET:CE	1:C:199:VAL:HG22	2.39	0.53
1:A:365:VAL:HG12	1:A:365:VAL:O	2.08	0.53
1:A:120:LYS:HB3	1:A:122:LEU:HD22	1.90	0.52
1:B:217:GLU:OE1	1:B:262:ARG:CB	2.57	0.52
1:A:75:ASN:C	1:A:76:PHE:CD1	2.82	0.52
1:A:21:LEU:C	1:A:22:ASN:OD1	2.47	0.52
1:C:122:LEU:N	1:C:123:PRO:HD3	2.25	0.52
2:E:2:A:C2'	2:E:2:A:N3	2.72	0.52
1:A:366:GLY:O	1:B:417:LYS:HB2	2.10	0.52
1:B:165:MET:CE	1:B:199:VAL:HG22	2.40	0.52
1:C:52:LEU:O	1:C:100:ILE:CD1	2.58	0.52
1:A:370:PHE:CD2	1:B:413:PRO:HD2	2.44	0.52
1:A:33:HIS:ND1	1:A:79:MET:HE1	2.21	0.52
1:B:94:VAL:HG13	1:B:128:ARG:H	1.73	0.52
1:B:430:ASN:HA	1:B:433:GLU:HB2	1.92	0.52
1:C:47:LEU:HD23	1:C:91:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HG23	1:B:302:ASN:HD22	1.74	0.52
1:C:203:ASN:HB2	3:C:523:HOH:O	2.10	0.52
1:C:354:ARG:HG2	1:C:399:ARG:NH1	2.25	0.52
1:A:98:SER:HA	1:A:122:LEU:O	2.10	0.52
1:A:94:VAL:HG13	1:A:128:ARG:H	1.74	0.52
1:A:230:LEU:CD2	1:A:243:LEU:HD21	2.40	0.52
1:A:347:ASP:HA	1:A:402:LEU:HD13	1.93	0.51
1:A:33:HIS:HE1	1:A:79:MET:HE2	1.61	0.51
1:B:35:LEU:HD22	1:B:39:PHE:HE2	1.75	0.51
1:C:356:LEU:HG	1:C:360:ILE:HD11	1.91	0.51
1:B:180:VAL:CG1	1:B:190:VAL:CG2	2.84	0.51
1:C:199:VAL:O	1:C:202:THR:HG22	2.10	0.51
1:A:307:THR:O	1:A:307:THR:OG1	2.18	0.51
1:A:336:LEU:HA	1:A:339:LEU:HD12	1.92	0.51
1:B:415:VAL:HA	1:B:421:ILE:HG23	1.91	0.51
1:A:17:VAL:HG12	1:A:184:PRO:HB2	1.93	0.51
1:B:130:PRO:HA	1:B:133:ILE:HD12	1.93	0.51
1:B:73:GLU:C	1:B:74:LEU:HG	2.28	0.51
1:A:284:GLU:OE1	1:A:321:LYS:NZ	2.40	0.51
1:B:266:THR:HB	1:B:333:LEU:HD21	1.92	0.51
1:B:266:THR:CB	1:B:333:LEU:HD21	2.40	0.51
1:C:236:GLU:O	1:C:240:LYS:HB2	2.11	0.51
1:A:267:VAL:CG2	1:A:268:ASN:H	2.24	0.50
1:B:1:MET:HB3	1:B:147:ASP:CG	2.32	0.50
1:B:61:GLU:OE1	1:B:65:ASN:ND2	2.44	0.50
1:A:103:GLU:CG	1:A:104:ASN:N	2.67	0.50
1:A:192:ILE:HG22	1:A:193:VAL:N	2.26	0.50
1:B:358:VAL:HG22	1:B:384:VAL:CG2	2.35	0.50
1:A:287:LEU:HD21	1:A:291:LYS:HE2	1.89	0.50
1:A:270:VAL:HG13	1:A:332:LYS:CB	2.40	0.50
1:C:9:GLY:HA3	1:C:14:TYR:OH	2.11	0.50
1:A:100:ILE:HD13	1:A:122:LEU:HD21	1.92	0.50
1:A:310:VAL:HG13	1:A:313:ASP:H	1.77	0.50
1:A:235:PHE:CZ	1:A:240:LYS:HG3	2.46	0.50
1:A:400:ASN:HB3	1:A:410:ASP:OD1	2.12	0.50
1:A:47:LEU:HD23	1:A:90:LYS:N	2.27	0.50
1:A:361:CYS:CB	1:A:451:LEU:HD21	2.40	0.50
1:C:415:VAL:CA	1:C:421:ILE:HG23	2.41	0.50
1:B:150:LEU:HD23	1:B:174:LYS:HB2	1.94	0.50
1:A:428:THR:HB	1:A:431:LYS:CB	2.42	0.49
1:A:57:VAL:HB	1:A:104:ASN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLU:OE2	1:B:259:TRP:CD1	2.64	0.49
1:B:267:VAL:CG2	1:B:268:ASN:HD22	2.09	0.49
1:B:294:TYR:CD2	1:B:311:LEU:HD11	2.47	0.49
1:B:415:VAL:HG23	1:B:421:ILE:CD1	2.42	0.49
1:C:294:TYR:CE2	1:C:311:LEU:HD11	2.47	0.49
1:B:110:GLU:CB	1:B:119:LEU:HD13	2.42	0.49
1:A:403:MET:CG	1:B:403:MET:HG2	2.42	0.49
1:C:151:VAL:HG12	1:C:173:ALA:HB1	1.93	0.49
1:A:235:PHE:CE1	1:A:240:LYS:CA	2.95	0.49
1:A:57:VAL:CG1	1:A:58:SER:N	2.69	0.49
1:C:387:TYR:CZ	1:C:391:ARG:HG2	2.40	0.49
1:C:415:VAL:HA	1:C:421:ILE:HG23	1.93	0.49
1:A:294:TYR:OH	1:A:309:LEU:HD23	2.13	0.49
1:A:398:PHE:HD2	1:A:435:PHE:HD2	1.50	0.49
1:C:266:THR:HB	1:C:333:LEU:CD2	2.43	0.49
1:C:1:MET:HB3	1:C:147:ASP:CG	2.33	0.49
1:B:21:LEU:HB3	1:B:192:ILE:HD11	1.95	0.49
1:A:199:VAL:O	1:A:202:THR:HG22	2.13	0.48
1:A:24:GLN:H	1:A:24:GLN:CD	2.15	0.48
1:A:130:PRO:HA	1:A:133:ILE:HD12	1.94	0.48
1:A:47:LEU:HB2	1:A:88:ILE:HG22	1.95	0.48
1:B:49:PRO:HD2	1:B:52:LEU:CD2	2.44	0.48
1:C:26:GLN:HG2	1:C:34:ALA:HA	1.96	0.48
1:C:53:VAL:HG22	1:C:102:CYS:SG	2.53	0.48
1:A:153:LEU:O	1:A:153:LEU:HD12	2.13	0.48
1:B:266:THR:O	1:B:270:VAL:HB	2.12	0.48
1:B:11:VAL:HB	1:B:66:LEU:HD21	1.96	0.48
1:C:387:TYR:O	1:C:391:ARG:CB	2.58	0.48
1:A:234:ILE:O	1:A:234:ILE:CD1	2.60	0.48
1:A:234:ILE:CG1	1:A:234:ILE:O	2.61	0.48
1:B:165:MET:HE2	1:B:199:VAL:HG22	1.96	0.48
1:C:111:LYS:CE	1:C:116:ARG:HB2	2.35	0.48
1:C:122:LEU:O	1:C:122:LEU:HG	2.13	0.48
1:A:267:VAL:CG1	1:B:407:LEU:HD12	2.44	0.48
1:A:232:PRO:CG	1:A:235:PHE:CD2	2.83	0.48
1:A:98:SER:HA	1:A:122:LEU:HB3	1.95	0.48
1:B:217:GLU:OE1	1:B:262:ARG:CD	2.62	0.48
1:B:389:ARG:HG2	1:B:396:MET:HG3	1.96	0.48
1:A:154:THR:HG23	1:A:178:ALA:HB3	1.96	0.47
1:A:303:PHE:HA	1:A:306:GLU:HG3	1.96	0.47
1:A:47:LEU:HG	1:A:90:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG12	1:A:276:LEU:HD21	1.96	0.47
1:B:232:PRO:O	1:B:235:PHE:HD1	1.95	0.47
1:A:297:TRP:HH2	1:B:50:ASP:HB3	1.80	0.47
1:A:153:LEU:HB2	1:A:161:VAL:HG13	1.95	0.47
1:A:33:HIS:ND1	1:A:79:MET:CE	2.71	0.47
1:B:20:GLU:HG3	1:B:20:GLU:O	2.15	0.47
1:C:48:ILE:HD11	1:C:53:VAL:CG1	2.44	0.47
1:B:178:ALA:HB2	1:B:192:ILE:HG22	1.97	0.47
1:B:57:VAL:CG2	1:B:58:SER:N	2.59	0.47
1:C:96:ILE:HA	1:C:124:TYR:O	2.15	0.47
1:B:231:ASN:N	1:B:232:PRO:HD3	2.30	0.47
1:C:180:VAL:CG1	2:E:2:A:C8	2.97	0.47
1:A:189:ILE:O	1:A:189:ILE:HG23	2.15	0.47
1:C:51:SER:HA	1:C:124:TYR:CD1	2.50	0.47
1:C:365:VAL:HG23	1:C:376:LYS:HD3	1.95	0.47
1:C:52:LEU:HA	2:E:1:A:N6	2.29	0.47
1:A:308:LEU:HA	1:A:308:LEU:HD13	1.73	0.47
1:A:38:LEU:C	1:A:38:LEU:HD23	2.35	0.47
1:B:28:THR:HG22	1:B:76:PHE:HZ	1.77	0.47
1:A:47:LEU:CD1	1:A:48:ILE:CG1	2.80	0.47
1:B:216:ASP:HB3	1:B:219:TYR:HD2	1.80	0.47
1:C:130:PRO:HA	1:C:133:ILE:HD12	1.97	0.47
1:A:101:GLN:O	1:A:102:CYS:HB3	2.14	0.47
1:B:362:LEU:HA	1:B:365:VAL:HG12	1.96	0.47
1:C:16:ILE:HB	1:C:186:LYS:HG2	1.97	0.47
1:A:354:ARG:HH21	1:A:384:VAL:HG23	1.80	0.47
1:C:242:VAL:HG22	1:C:289:LYS:HD2	1.97	0.47
1:B:182:GLY:HA2	2:D:2:A:O2'	2.15	0.47
1:A:266:THR:HB	1:A:333:LEU:HD21	1.97	0.46
1:A:11:VAL:HG11	1:A:67:VAL:HA	1.97	0.46
1:A:1:MET:HB2	1:A:147:ASP:CG	2.35	0.46
1:B:154:THR:HG21	1:B:178:ALA:O	2.15	0.46
1:A:66:LEU:HD12	1:A:66:LEU:C	2.35	0.46
1:A:214:ASN:HD22	1:B:218:ARG:HD3	1.79	0.46
1:A:249:THR:CB	1:A:283:LEU:HD11	2.45	0.46
1:B:21:LEU:CB	1:B:192:ILE:CG1	2.89	0.46
1:B:411:MET:HE1	1:B:425:LYS:HB2	1.97	0.46
1:C:165:MET:HE3	1:C:199:VAL:HG22	1.96	0.46
1:C:407:LEU:CD2	1:C:407:LEU:N	2.73	0.46
1:A:11:VAL:HG21	1:A:67:VAL:HG23	1.97	0.46
1:A:81:GLU:C	1:A:83:MET:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LEU:HD13	1:B:368:GLY:O	2.14	0.46
1:C:54:LYS:HA	1:C:54:LYS:HD2	1.74	0.46
1:C:83:MET:HA	1:C:86:VAL:HG12	1.98	0.46
1:B:217:GLU:CD	1:B:262:ARG:HD2	2.36	0.46
1:B:283:LEU:HD11	1:B:314:LEU:HD23	1.98	0.46
1:C:264:GLY:CA	1:C:348:LYS:HD2	2.46	0.46
1:B:266:THR:CB	1:B:333:LEU:CD2	2.93	0.46
1:A:98:SER:C	1:A:122:LEU:HB3	2.37	0.45
1:A:267:VAL:HG12	1:B:407:LEU:HD12	1.97	0.45
1:C:121:ARG:HB3	1:C:123:PRO:HD3	1.98	0.45
1:A:151:VAL:HG12	1:A:173:ALA:HB1	1.98	0.45
1:A:55:ASP:HB3	1:A:102:CYS:HB3	1.98	0.45
1:B:217:GLU:CD	1:B:259:TRP:HA	2.37	0.45
1:C:28:THR:HG21	1:C:33:HIS:HB3	1.98	0.45
1:A:309:LEU:O	1:B:131:ILE:CD1	2.64	0.45
1:A:64:LYS:HE3	1:A:84:ASN:HA	1.98	0.45
1:B:287:LEU:CD2	1:B:318:LEU:HD11	2.46	0.45
1:A:266:THR:O	1:A:270:VAL:HG23	2.17	0.45
1:A:8:ALA:CB	1:A:48:ILE:HG23	2.46	0.45
1:A:347:ASP:CA	1:A:402:LEU:HD13	2.47	0.45
1:A:6:TYR:CE1	1:A:46:ALA:HB2	2.52	0.45
1:C:100:ILE:HG23	1:C:118:VAL:CG1	2.47	0.45
1:C:391:ARG:HA	1:C:391:ARG:HD3	1.62	0.45
1:A:237:GLU:HG2	1:A:238:GLU:N	2.32	0.44
1:B:404:HIS:N	1:B:404:HIS:CD2	2.83	0.44
1:A:181:MET:CG	2:D:1:A:N1	2.75	0.44
1:B:444:PHE:HA	1:B:447:ILE:HD12	1.98	0.44
1:C:155:HIS:CE1	2:E:2:A:C8	3.05	0.44
1:A:403:MET:HG3	1:B:403:MET:HG2	2.00	0.44
1:C:408:SER:C	1:C:410:ASP:H	2.20	0.44
1:C:408:SER:C	1:C:410:ASP:N	2.70	0.44
1:A:28:THR:CG2	1:A:33:HIS:ND1	2.79	0.44
1:B:217:GLU:OE1	1:B:262:ARG:NE	2.51	0.44
1:B:21:LEU:CB	1:B:192:ILE:HD11	2.47	0.44
1:C:234:ILE:HG21	1:C:302:ASN:HD22	1.82	0.44
1:A:259:TRP:HH2	1:B:432:ILE:HD13	1.83	0.44
1:C:401:THR:O	1:C:405:GLY:N	2.49	0.44
1:C:341:ILE:HD11	1:C:440:LEU:HD23	2.00	0.44
1:A:287:LEU:HD23	1:A:291:LYS:HE3	2.00	0.44
1:B:362:LEU:O	1:B:365:VAL:HG12	2.18	0.44
1:B:16:ILE:CD1	1:B:74:LEU:HD21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:O	1:A:314:LEU:CD1	2.66	0.43
1:B:361:CYS:HB2	1:B:451:LEU:HD22	2.00	0.43
1:A:237:GLU:HA	1:A:240:LYS:HB3	2.00	0.43
1:B:47:LEU:HD12	1:B:140:ILE:HD11	2.00	0.43
1:C:97:ALA:HB3	1:C:124:TYR:HB3	2.00	0.43
1:A:370:PHE:CE2	1:B:415:VAL:HB	2.52	0.43
1:A:215:LEU:HD11	1:A:323:LEU:HD22	2.00	0.43
1:A:350:LEU:HD23	1:A:440:LEU:HD22	1.99	0.43
1:A:365:VAL:CG1	1:A:376:LYS:CD	2.94	0.43
1:B:445:ASP:HA	1:B:448:VAL:HG22	2.00	0.43
1:B:266:THR:HB	1:B:333:LEU:HD23	2.00	0.43
1:A:230:LEU:HD21	1:A:243:LEU:HD11	2.00	0.43
1:B:21:LEU:HD22	1:B:22:ASN:N	2.34	0.43
1:B:230:LEU:CB	1:B:247:LYS:HG3	2.49	0.43
1:A:350:LEU:CD2	1:A:440:LEU:HD13	2.49	0.43
1:B:180:VAL:HG13	1:B:190:VAL:CG2	2.35	0.43
1:B:165:MET:HE3	1:B:199:VAL:CG2	2.48	0.43
1:A:428:THR:HB	1:A:431:LYS:HB3	1.99	0.43
1:B:266:THR:OG1	1:B:333:LEU:HD21	2.19	0.43
1:C:404:HIS:HB3	1:C:408:SER:HB2	2.01	0.43
1:A:362:LEU:HD12	1:A:370:PHE:CE1	2.54	0.43
1:A:46:ALA:N	1:A:87:GLU:O	2.42	0.43
1:B:350:LEU:HD13	1:B:402:LEU:HD12	2.01	0.43
1:A:270:VAL:HG21	1:A:333:LEU:HG	2.01	0.42
1:A:409:THR:HA	1:B:370:PHE:O	2.19	0.42
1:B:66:LEU:O	1:B:66:LEU:HD23	2.18	0.42
1:B:181:MET:SD	2:D:3:A:C5	3.12	0.42
1:B:217:GLU:CD	1:B:262:ARG:HE	2.22	0.42
1:C:337:LEU:HD11	1:C:353:ALA:HB2	2.01	0.42
1:C:361:CYS:HB2	1:C:451:LEU:HD22	2.02	0.42
1:C:387:TYR:CZ	1:C:391:ARG:HG3	2.54	0.42
1:A:21:LEU:CD1	1:A:192:ILE:HB	2.50	0.42
1:B:293:PHE:CB	1:B:300:HIS:CD2	3.00	0.42
1:C:98:SER:HA	1:C:122:LEU:HA	2.01	0.42
1:C:4:LEU:HB2	1:C:41:PRO:HG3	2.01	0.42
1:C:444:PHE:HA	1:C:447:ILE:HD12	2.01	0.42
1:A:21:LEU:HD12	1:A:192:ILE:HB	2.01	0.42
1:B:16:ILE:HD11	1:B:74:LEU:HD21	2.02	0.42
1:B:277:LYS:HD2	1:B:324:LEU:HD23	2.01	0.42
1:C:52:LEU:HD12	1:C:100:ILE:HD13	2.01	0.42
1:A:230:LEU:O	1:A:247:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:VAL:CG1	1:C:268:ASN:H	2.32	0.42
1:A:24:GLN:N	1:A:24:GLN:CD	2.73	0.42
1:B:309:LEU:HD12	1:B:310:VAL:H	1.83	0.42
1:C:264:GLY:HA3	1:C:348:LYS:HD2	2.00	0.42
1:C:62:CYS:HA	1:C:105:GLY:O	2.20	0.42
1:A:445:ASP:O	1:A:449:ASN:HB2	2.20	0.42
1:A:302:ASN:C	1:A:304:GLN:H	2.23	0.42
1:B:217:GLU:HG3	1:B:259:TRP:CD1	2.54	0.42
1:C:154:THR:HG23	1:C:178:ALA:HB3	2.00	0.42
1:C:320:VAL:HG23	1:C:323:LEU:HD22	2.02	0.42
1:A:285:GLU:O	1:A:288:GLU:CA	2.68	0.41
1:A:294:TYR:CD2	1:A:311:LEU:HD11	2.55	0.41
1:B:414:ASN:O	1:B:415:VAL:CG1	2.67	0.41
1:C:354:ARG:HH22	1:C:381:ASN:ND2	2.03	0.41
1:A:20:GLU:HB3	1:A:191:ASN:HA	2.03	0.41
1:A:243:LEU:HD23	1:A:243:LEU:C	2.40	0.41
1:A:307:THR:HB	1:B:129:SER:HB2	2.02	0.41
1:B:217:GLU:CD	1:B:262:ARG:CD	2.88	0.41
1:B:310:VAL:CG1	1:B:313:ASP:CB	2.95	0.41
1:A:365:VAL:HG12	1:A:376:LYS:NZ	2.35	0.41
1:C:236:GLU:CD	1:C:237:GLU:N	2.73	0.41
1:A:237:GLU:O	1:A:240:LYS:HB3	2.21	0.41
1:B:407:LEU:N	1:B:407:LEU:CD1	2.82	0.41
1:C:17:VAL:HG22	1:C:190:VAL:HG12	2.02	0.41
1:A:131:ILE:HD13	1:B:307:THR:OG1	2.20	0.41
1:C:52:LEU:HA	2:E:1:A:H62	1.83	0.41
1:A:49:PRO:HA	1:A:91:ILE:HG13	2.01	0.41
1:B:308:LEU:HG	1:B:308:LEU:H	1.67	0.41
1:B:56:ASN:N	1:B:56:ASN:OD1	2.54	0.41
1:C:361:CYS:O	1:C:364:LYS:HB2	2.21	0.41
1:B:416:ASP:OD1	1:B:417:LYS:N	2.54	0.41
1:C:102:CYS:HA	1:C:107:PRO:HA	2.03	0.41
1:A:120:LYS:HA	1:A:122:LEU:HD22	2.03	0.41
1:A:267:VAL:CG2	1:A:268:ASN:N	2.82	0.41
1:B:71:ALA:O	1:B:76:PHE:HB3	2.21	0.41
1:A:365:VAL:HG11	1:A:376:LYS:CG	2.48	0.40
1:C:215:LEU:HD23	1:C:343:ALA:HB2	2.03	0.40
1:C:224:SER:OG	1:C:251:VAL:CG1	2.69	0.40
1:C:215:LEU:HD23	1:C:343:ALA:CB	2.51	0.40
1:B:362:LEU:O	1:B:367:GLY:HA2	2.22	0.40
1:A:60:GLU:HB3	1:A:88:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:TYR:HB3	1:C:152:ASP:HB3	2.02	0.40
1:A:428:THR:HB	1:A:431:LYS:HB2	2.02	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	452/454 (100%)	392 (87%)	52 (12%)	8 (2%)	8 33
1	B	452/454 (100%)	404 (89%)	43 (10%)	5 (1%)	14 45
1	C	452/454 (100%)	412 (91%)	37 (8%)	3 (1%)	22 56
All	All	1356/1362 (100%)	1208 (89%)	132 (10%)	16 (1%)	13 43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	B	233	THR
1	A	47	LEU
1	A	78	GLY
1	A	415	VAL
1	B	306	GLU
1	C	366	GLY
1	C	409	THR
1	A	46	ALA
1	B	104	ASN
1	A	105	GLY
1	C	122	LEU
1	B	57	VAL
1	A	267	VAL
1	A	123	PRO

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Mol	Chain	Res	Type
1	B	122	LEU

5.3.2 Protein sidechains

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	407/407 (100%)	387 (95%)	20 (5%)	25 57
1	B	407/407 (100%)	383 (94%)	24 (6%)	19 50
1	C	407/407 (100%)	388 (95%)	19 (5%)	26 58
All	All	1221/1221 (100%)	1158 (95%)	63 (5%)	23 54

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	PHE
1	A	181	MET
1	A	183	MET
1	A	223	TYR
1	A	249	THR
1	A	262	ARG
1	A	273	MET
1	A	283	LEU
1	A	285	GLU
1	A	303	PHE
1	A	307	THR
1	A	308	LEU
1	A	310	VAL
1	A	329	ASP
1	A	354	ARG
1	A	361	CYS
1	A	448	VAL
1	A	449	ASN
1	A	450	PHE
1	A	451	LEU
1	B	20	GLU

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Mol	Chain	Res	Type
1	B	21	LEU
1	B	22	ASN
1	B	24	GLN
1	B	30	PHE
1	B	55	ASP
1	B	62	CYS
1	B	118	VAL
1	B	216	ASP
1	B	235	PHE
1	B	239	GLU
1	B	262	ARG
1	B	270	VAL
1	B	273	MET
1	B	308	LEU
1	B	310	VAL
1	B	325	ILE
1	B	329	ASP
1	B	354	ARG
1	B	361	CYS
1	B	390	LEU
1	B	413	PRO
1	B	420	ASN
1	B	422	THR
1	C	30	PHE
1	C	51	SER
1	C	52	LEU
1	C	189	ILE
1	C	237	GLU
1	C	244	THR
1	C	249	THR
1	C	250	ASP
1	C	270	VAL
1	C	273	MET
1	C	274	ASN
1	C	286	ASP
1	C	298	GLU
1	C	329	ASP
1	C	361	CYS
1	C	391	ARG
1	C	418	ASP
1	C	421	ILE
1	C	422	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	18	ASN
1	A	24	GLN
1	A	33	HIS
1	A	69	ASN
1	A	75	ASN
1	A	214	ASN
1	A	252	ASN
1	A	274	ASN
1	A	449	ASN
1	B	69	ASN
1	B	166	ASN
1	B	172	ASN
1	B	256	ASN
1	B	263	ASN
1	B	268	ASN
1	B	300	HIS
1	B	302	ASN
1	B	374	ASN
1	B	404	HIS
1	C	26	GLN
1	C	155	HIS
1	C	274	ASN
1	C	381	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	3/4 (75%)	3 (100%)	1 (33%)
2	E	1/4 (25%)	1 (100%)	0
All	All	4/8 (50%)	4 (100%)	1 (25%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	2	A
2	D	3	A
2	D	4	A
2	E	2	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	3	A

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	454/454 (100%)	0.29	17 (3%) 41 21	94, 142, 199, 226	0
1	B	454/454 (100%)	0.27	22 (4%) 30 14	79, 135, 199, 213	0
1	C	454/454 (100%)	-0.05	2 (0%) 92 85	58, 106, 147, 166	0
2	D	4/4 (100%)	0.75	0 100 100	187, 188, 192, 194	0
2	E	2/4 (50%)	0.34	0 100 100	110, 110, 110, 112	0
All	All	1368/1370 (99%)	0.17	41 (2%) 50 27	58, 126, 195, 226	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	ARG	6.8
1	A	75	ASN	6.3
1	B	123	PRO	5.3
1	C	233	THR	4.8
1	A	76	PHE	4.3
1	A	120	LYS	4.3
1	A	47	LEU	4.0
1	B	95	GLY	3.9
1	C	454	ALA	3.8
1	B	56	ASN	3.4
1	B	75	ASN	3.4
1	A	192	ILE	3.3
1	B	47	LEU	3.3
1	B	116	ARG	3.2
1	A	48	ILE	3.1
1	A	116	ARG	3.0
1	B	77	ALA	3.0
1	B	232	PRO	2.8
1	A	21	LEU	2.8
1	B	82	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	233	THR	2.7
1	B	44	VAL	2.7
1	B	54	LYS	2.6
1	A	184	PRO	2.4
1	B	39	PHE	2.4
1	B	395	LEU	2.4
1	A	2	LYS	2.4
1	B	454	ALA	2.3
1	A	79	MET	2.3
1	A	325	ILE	2.2
1	A	63	TYR	2.2
1	B	103	GLU	2.2
1	B	239	GLU	2.2
1	B	76	PHE	2.1
1	B	84	ASN	2.1
1	B	88	ILE	2.1
1	A	187	ASP	2.1
1	B	5	PHE	2.0
1	B	421	ILE	2.0
1	A	77	ALA	2.0
1	B	63	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.