Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 05:18 PM EST

PDB ID	:	2P9L
Title	:	Crystal Structure of bovine Arp2/3 complex
Authors	:	Nolen, B.J.; Pollard, T.D.
Deposited on	:	2007-03-26
Resolution	:	2.65 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 (i) 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 (1)) were used in the production of this report:

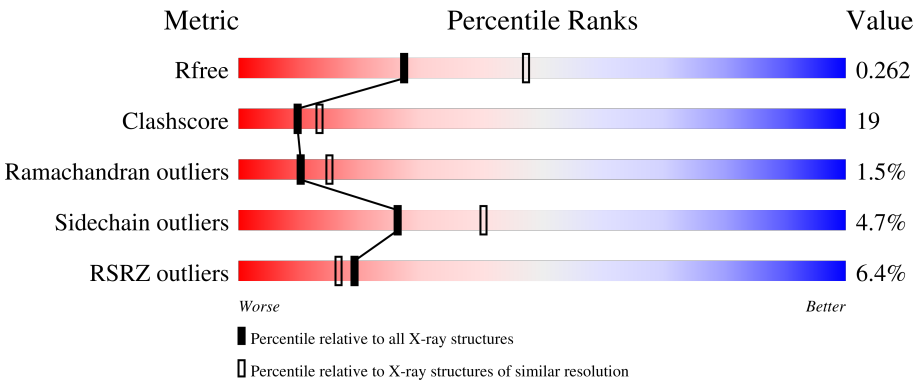
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	6% 64% 28% • 5%
2	B	394	7% 30% 16% • 49%
3	C	372	2% 63% 27% • 8%
4	D	300	2% 66% 24% • 8%
5	E	178	13% 48% 43% 5% • •

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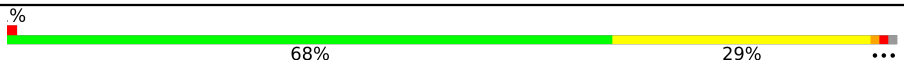
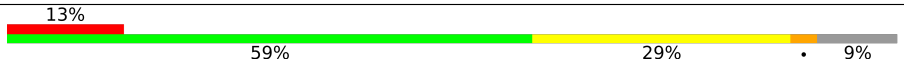
Mol	Chain	Length	Quality of chain
6	F	168	
7	G	151	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13500 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 Actin-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	3179	2043	526	595	15	0	0	0

- Molecule 2 is a protein called Actin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	201	1523	972	263	284	4	0	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	341	2648	1680	464	485	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	VAL	ILE	conflict	UNP Q58CQ2

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	277	2237	1422	389	418	8	0	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	173	1404	900	235	260	9	0	0	0

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	166	1360	869	238	244	9	0	0	0

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	137	1026	644	175	204	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ASP	GLY	conflict	UNP Q3SYX9
G	28	ASP	GLU	conflict	UNP Q3SYX9

- Molecule 8 is water.

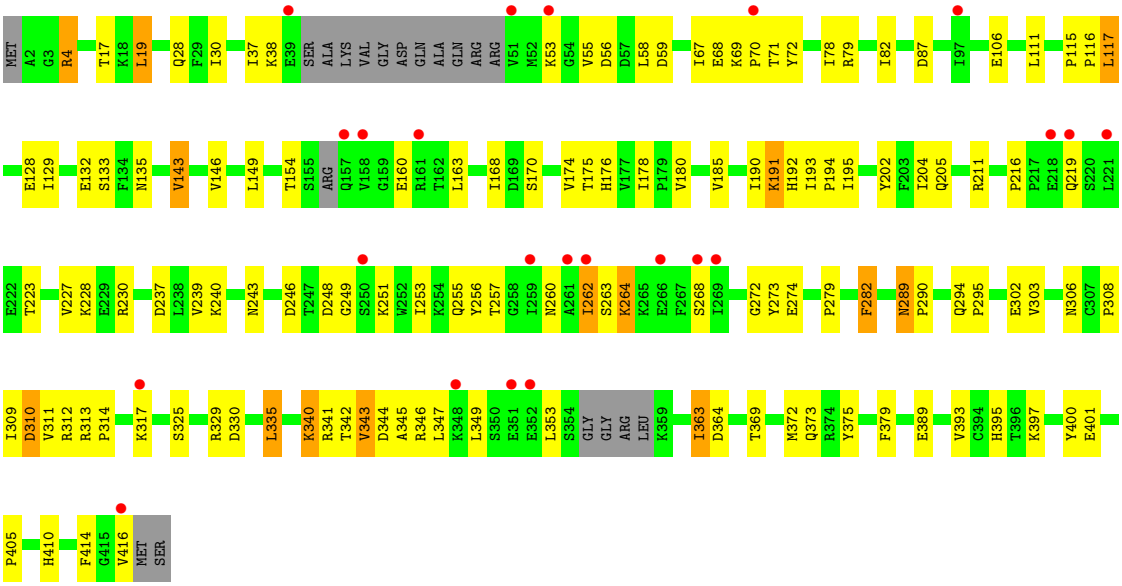
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	27	27	27	0	0
8	B	6	6	6	0	0
8	C	39	39	39	0	0
8	D	24	24	24	0	0
8	E	1	1	1	0	0
8	F	25	25	25	0	0
8	G	1	1	1	0	0

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.

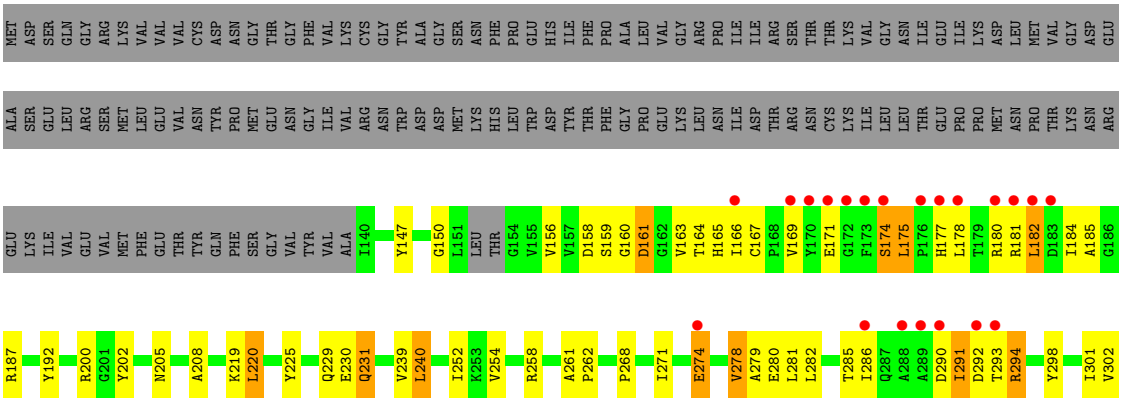
- Molecule 1: Actin-like protein 3

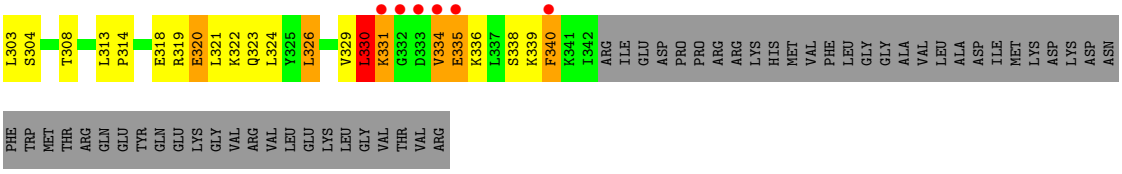
Chain A:



- Molecule 2: Actin-like protein 2

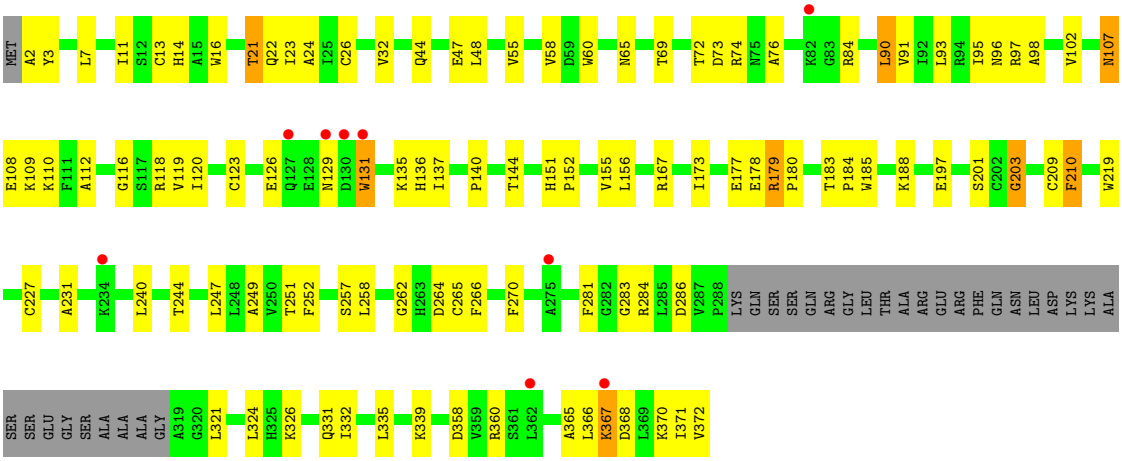
Chain B:





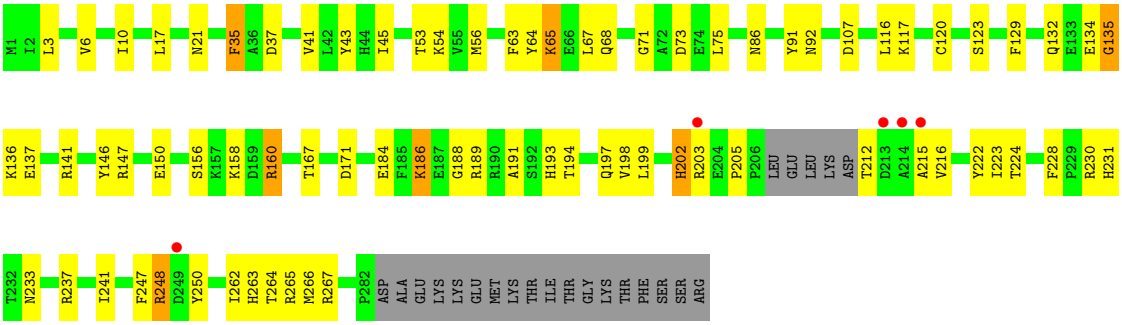
- Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:



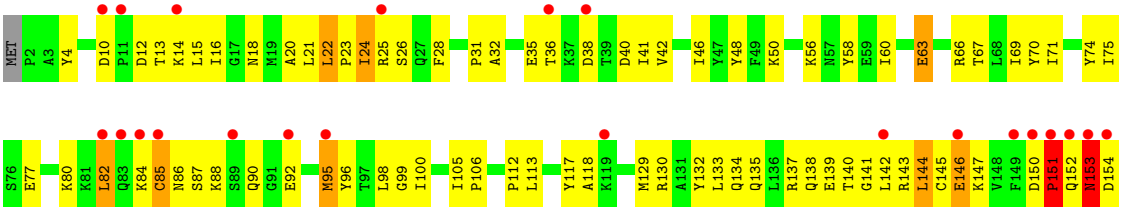
- Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:



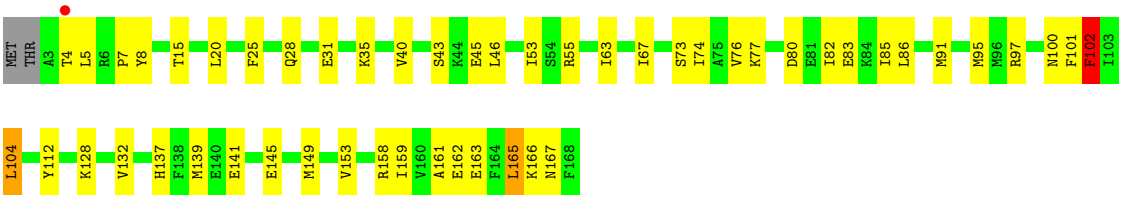
- Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:



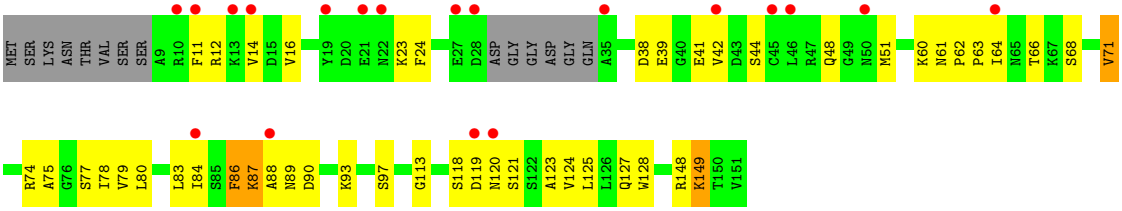
• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



• Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.06Å 128.06Å 204.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 45.58 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.8 (30.00-2.65) 89.6 (45.58-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.266 0.220 , 0.262	Depositor DCC
R_{free} test set	4094 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 64.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13500	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 (i)

5.1 Standard geometry (i)

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	0.38	0/3259	0.61	0/4425
2	B	0.35	0/1548	0.62	0/2099
3	C	0.38	0/2717	0.67	1/3688 (0.0%)
4	D	0.38	0/2285	0.61	0/3084
5	E	0.34	0/1437	0.62	0/1938
6	F	0.40	0/1382	0.63	0/1853
7	G	0.32	0/1038	0.53	0/1400
All	All	0.37	0/13666	0.62	1/18487 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	11	ILE	N-CA-C	-6.47	93.54	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3179	0	3107	113	0
2	B	1523	0	1487	76	0
3	C	2648	0	2602	90	0
4	D	2237	0	2202	68	0
5	E	1404	0	1406	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1360	0	1399	47	0
7	G	1026	0	1019	56	0
8	A	27	0	0	0	0
8	B	6	0	0	0	0
8	C	39	0	0	2	0
8	D	24	0	0	2	0
8	E	1	0	0	0	0
8	F	25	0	0	0	0
8	G	1	0	0	0	0
All	All	13500	0	13222	512	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 19.

All (512) 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)
6:F:4:THR:HG23	6:F:55:ARG:HE	1.28	0.96
5:E:25:ARG:HG3	5:E:35:GLU:HB3	1.48	0.94
3:C:284:ARG:HD3	3:C:286:ASP:O	1.67	0.94
7:G:87:LYS:HE3	7:G:87:LYS:H	1.33	0.94
2:B:291:ILE:HG22	2:B:292:ASP:H	1.34	0.93
2:B:205:ASN:HD22	2:B:208:ALA:H	1.18	0.92
1:A:363:ILE:HD13	1:A:363:ILE:H	1.36	0.91
5:E:95:MET:HG2	5:E:141:GLY:O	1.73	0.88
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.55	0.87
3:C:201:SER:HB3	7:G:149:LYS:HE3	1.56	0.87
4:D:65:LYS:NZ	4:D:65:LYS:HA	1.90	0.86
1:A:257:THR:HG22	1:A:268:SER:HB3	1.59	0.85
3:C:183:THR:HG22	3:C:185:TRP:H	1.39	0.84
1:A:389:GLU:OE1	1:A:414:PHE:HB2	1.79	0.82
1:A:163:LEU:HG	1:A:416:VAL:HG13	1.62	0.81
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.46	0.81
5:E:139:GLU:O	5:E:142:LEU:HD23	1.83	0.79
1:A:260:ASN:O	1:A:264:LYS:HA	1.83	0.79
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.65	0.78
2:B:160:GLY:O	2:B:185:ALA:HB1	1.83	0.78
2:B:182:LEU:HG	2:B:281:LEU:HD12	1.65	0.78
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.65	0.78
5:E:24:ILE:O	5:E:24:ILE:HG13	1.83	0.78
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:ARG:HB3	4:D:160:ARG:HH11	1.47	0.77
2:B:165:HIS:CD2	2:B:181:ARG:HG2	2.19	0.77
2:B:205:ASN:ND2	2:B:208:ALA:H	1.82	0.76
6:F:4:THR:HG23	6:F:55:ARG:NE	2.01	0.76
7:G:23:LYS:HG2	7:G:24:PHE:H	1.49	0.75
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.68	0.75
1:A:67:ILE:HG22	1:A:68:GLU:HG2	1.66	0.75
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.68	0.74
5:E:87:SER:HA	5:E:153:ASN:ND2	2.01	0.74
3:C:14:HIS:H	3:C:331:GLN:HE22	1.34	0.74
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.70	0.74
2:B:229:GLN:HE21	6:F:40:VAL:HG12	1.51	0.74
4:D:65:LYS:HA	4:D:65:LYS:HZ3	1.54	0.73
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.69	0.73
2:B:322:LYS:HB3	7:G:16:VAL:HG11	1.72	0.72
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.53	0.72
1:A:223:THR:O	1:A:227:VAL:HG23	1.88	0.72
2:B:229:GLN:HE21	6:F:40:VAL:CG1	2.02	0.72
1:A:257:THR:HG22	1:A:268:SER:CB	2.19	0.72
1:A:55:VAL:CG1	1:A:58:LEU:HD12	2.20	0.71
6:F:163:GLU:HA	6:F:166:LYS:HE3	1.71	0.71
7:G:23:LYS:HG2	7:G:24:PHE:N	2.05	0.71
7:G:66:THR:HG21	7:G:71:VAL:HG21	1.72	0.71
3:C:367:LYS:HD2	3:C:368:ASP:N	2.05	0.70
7:G:80:LEU:O	7:G:84:ILE:HD13	1.92	0.70
3:C:367:LYS:HD2	3:C:367:LYS:C	2.12	0.70
2:B:291:ILE:HG22	2:B:292:ASP:N	2.07	0.69
3:C:358:ASP:OD1	3:C:360:ARG:HG2	1.92	0.69
1:A:347:LEU:HD22	1:A:363:ILE:HD12	1.74	0.69
5:E:86:ASN:HB3	5:E:154:ASP:OD2	1.93	0.69
5:E:88:LYS:N	5:E:153:ASN:HD21	1.91	0.69
4:D:189:ARG:HH22	4:D:197:GLN:NE2	1.92	0.68
1:A:55:VAL:HG12	1:A:55:VAL:O	1.93	0.68
1:A:363:ILE:H	1:A:363:ILE:CD1	2.07	0.67
7:G:38:ASP:O	7:G:42:VAL:HG23	1.93	0.67
2:B:165:HIS:HD2	2:B:181:ARG:HG2	1.60	0.67
5:E:96:TYR:O	5:E:100:ILE:HG12	1.94	0.67
7:G:87:LYS:HE3	7:G:87:LYS:N	2.09	0.67
7:G:60:LYS:HG2	7:G:61:ASN:HD22	1.60	0.67
3:C:107:ASN:ND2	3:C:109:LYS:H	1.93	0.67
1:A:55:VAL:HG13	1:A:58:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:162:GLU:O	6:F:166:LYS:HB3	1.95	0.66
2:B:182:LEU:HD11	2:B:278:VAL:H	1.60	0.66
3:C:2:ALA:N	8:C:392:HOH:O	2.29	0.66
5:E:153:ASN:ND2	5:E:154:ASP:H	1.93	0.66
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.78	0.66
5:E:84:LYS:O	5:E:85:CYS:HB3	1.95	0.66
5:E:146:GLU:O	5:E:146:GLU:HG2	1.96	0.66
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.78	0.66
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.32	0.65
3:C:371:ILE:HG22	3:C:372:VAL:CG2	2.27	0.65
5:E:22:LEU:HD23	5:E:41:ILE:HD13	1.78	0.65
1:A:340:LYS:O	1:A:343:VAL:HG12	1.97	0.64
4:D:150:GLU:HG2	4:D:167:THR:HA	1.80	0.64
1:A:78:ILE:O	1:A:79:ARG:HD2	1.98	0.64
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.29	0.64
1:A:311:VAL:C	1:A:314:PRO:HD2	2.18	0.64
2:B:274:GLU:OE1	2:B:274:GLU:HA	1.97	0.64
4:D:263:HIS:HD2	4:D:266:MET:HE3	1.62	0.63
4:D:262:ILE:HG22	4:D:266:MET:CE	2.27	0.63
4:D:65:LYS:HA	4:D:65:LYS:HZ2	1.60	0.63
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.28	0.63
7:G:149:LYS:HZ3	7:G:149:LYS:HB2	1.64	0.63
4:D:262:ILE:HG22	4:D:266:MET:HE2	1.78	0.63
2:B:229:GLN:NE2	6:F:40:VAL:HB	2.12	0.62
7:G:87:LYS:C	7:G:89:ASN:H	2.03	0.62
7:G:118:SER:HB3	7:G:121:SER:OG	2.00	0.62
7:G:51:MET:HG3	7:G:87:LYS:NZ	2.15	0.62
2:B:174:SER:C	2:B:175:LEU:HD23	2.20	0.62
2:B:182:LEU:HD11	2:B:278:VAL:N	2.13	0.62
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.82	0.62
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.64	0.61
2:B:230:GLU:OE2	6:F:35:LYS:HE2	2.00	0.61
1:A:163:LEU:HG	1:A:416:VAL:CG1	2.30	0.61
1:A:211:ARG:HH11	5:E:159:TRP:HZ3	1.46	0.61
5:E:87:SER:HA	5:E:153:ASN:CG	2.21	0.61
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.82	0.61
5:E:154:ASP:O	5:E:156:PRO:HD3	2.01	0.61
4:D:228:PHE:H	4:D:231:HIS:HD2	1.46	0.61
2:B:205:ASN:HD22	2:B:208:ALA:N	1.94	0.61
1:A:343:VAL:CG2	1:A:363:ILE:HG13	2.31	0.61
1:A:17:THR:HG22	1:A:19:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HE3	1:A:364:ASP:OD1	2.00	0.60
1:A:116:PRO:HG2	1:A:178:ILE:HD13	1.82	0.60
5:E:146:GLU:OE2	5:E:147:LYS:HG2	2.01	0.60
2:B:169:VAL:HA	2:B:174:SER:HA	1.81	0.60
4:D:215:ALA:O	4:D:222:TYR:OH	2.20	0.60
5:E:159:TRP:HA	5:E:159:TRP:CE3	2.36	0.60
4:D:86:ASN:HB3	8:D:316:HOH:O	2.01	0.60
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.66	0.60
2:B:175:LEU:CD1	2:B:178:LEU:HD12	2.32	0.60
5:E:139:GLU:HA	5:E:139:GLU:OE1	2.01	0.60
3:C:44:GLN:NE2	3:C:47:GLU:HG3	2.17	0.59
3:C:144:THR:H	6:F:28:GLN:NE2	1.99	0.59
5:E:74:TYR:OH	5:E:98:LEU:HD12	2.02	0.59
2:B:147:TYR:O	2:B:150:GLY:N	2.36	0.59
3:C:107:ASN:HD22	3:C:108:GLU:N	2.00	0.59
3:C:72:THR:HA	3:C:98:ALA:HB1	1.83	0.59
4:D:202:HIS:CG	4:D:203:ARG:N	2.71	0.59
1:A:262:ILE:HG22	1:A:263:SER:N	2.17	0.59
2:B:182:LEU:HG	2:B:281:LEU:CD1	2.32	0.59
3:C:135:LYS:HD3	3:C:173:ILE:CD1	2.33	0.58
3:C:90:LEU:HD23	3:C:91:VAL:H	1.69	0.58
5:E:159:TRP:HA	5:E:159:TRP:HE3	1.68	0.58
1:A:246:ASP:OD1	5:E:50:LYS:HE3	2.03	0.58
7:G:44:SER:O	7:G:48:GLN:HG3	2.03	0.58
1:A:4:ARG:HH11	1:A:4:ARG:CB	2.14	0.58
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.02	0.58
7:G:87:LYS:O	7:G:89:ASN:N	2.36	0.58
1:A:211:ARG:HD2	5:E:159:TRP:CZ3	2.39	0.58
4:D:186:LYS:O	4:D:186:LYS:HG3	2.02	0.58
4:D:189:ARG:HH22	4:D:197:GLN:HE21	1.51	0.58
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.39	0.57
6:F:149:MET:O	6:F:153:VAL:HG23	2.05	0.57
5:E:13:THR:HG21	5:E:22:LEU:CD1	2.35	0.57
2:B:158:ASP:HA	2:B:304:SER:O	2.03	0.57
6:F:80:ASP:OD1	6:F:83:GLU:HG3	2.04	0.57
4:D:202:HIS:CG	4:D:203:ARG:H	2.23	0.57
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.87	0.57
1:A:194:PRO:C	1:A:195:ILE:HD12	2.25	0.57
1:A:194:PRO:O	1:A:195:ILE:HD12	2.04	0.57
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.40	0.57
1:A:347:LEU:CD2	1:A:363:ILE:HD12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:67:LEU:HD13	4:D:120:CYS:O	2.05	0.57
7:G:11:PHE:CE1	7:G:12:ARG:HG3	2.39	0.57
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.87	0.56
4:D:228:PHE:H	4:D:231:HIS:CD2	2.22	0.56
5:E:10:ASP:C	5:E:12:ASP:H	2.09	0.56
5:E:20:ALA:HB1	5:E:22:LEU:HD13	1.87	0.56
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.87	0.56
2:B:291:ILE:HD12	2:B:291:ILE:N	2.20	0.56
3:C:201:SER:CB	7:G:149:LYS:HE3	2.33	0.56
5:E:71:ILE:O	5:E:75:ILE:HG13	2.05	0.56
6:F:163:GLU:O	6:F:167:ASN:ND2	2.39	0.56
1:A:82:ILE:HD12	1:A:115:PRO:HG3	1.88	0.56
1:A:311:VAL:O	1:A:314:PRO:HD2	2.06	0.56
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.36	0.56
1:A:69:LYS:HB3	1:A:72:TYR:HB2	1.87	0.56
5:E:24:ILE:O	5:E:24:ILE:CG1	2.53	0.56
2:B:163:VAL:HG22	2:B:164:THR:N	2.20	0.55
3:C:32:VAL:HB	3:C:48:LEU:HB2	1.88	0.55
5:E:150:ASP:O	5:E:152:GLN:N	2.39	0.55
3:C:240:LEU:HD23	3:C:270:PHE:CE2	2.41	0.55
2:B:159:SER:HB3	2:B:308:THR:HG23	1.88	0.55
1:A:170:SER:OG	1:A:325:SER:HB2	2.06	0.55
6:F:74:ILE:HD13	6:F:139:MET:HG2	1.88	0.55
3:C:281:PHE:CE2	3:C:283:GLY:HA2	2.42	0.55
5:E:58:TYR:CD1	5:E:168:PHE:HZ	2.23	0.55
1:A:174:VAL:HG12	1:A:175:THR:N	2.22	0.55
1:A:343:VAL:HG23	1:A:346:ARG:HH21	1.71	0.55
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.21	0.55
1:A:211:ARG:NH1	5:E:159:TRP:HZ3	2.05	0.55
1:A:248:ASP:OD1	1:A:251:LYS:HD3	2.07	0.55
5:E:139:GLU:OE1	5:E:142:LEU:HD21	2.07	0.55
5:E:153:ASN:O	5:E:155:LYS:HG3	2.07	0.55
1:A:343:VAL:HG22	1:A:363:ILE:HG13	1.89	0.54
4:D:35:PHE:N	4:D:35:PHE:CD2	2.76	0.54
1:A:87:ASP:OD2	4:D:267:ARG:HD2	2.07	0.54
5:E:88:LYS:O	5:E:92:GLU:HG3	2.08	0.54
1:A:309:ILE:HA	1:A:312:ARG:NE	2.22	0.54
3:C:90:LEU:HD23	3:C:91:VAL:N	2.21	0.54
4:D:141:ARG:HH21	4:D:212:THR:CG2	2.20	0.54
4:D:160:ARG:HB3	4:D:160:ARG:NH1	2.21	0.54
2:B:323:GLN:HG3	7:G:16:VAL:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:87:LYS:N	7:G:87:LYS:CD	2.70	0.53
2:B:323:GLN:HG3	7:G:16:VAL:HG21	1.91	0.53
5:E:14:LYS:HA	5:E:14:LYS:HE2	1.90	0.53
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.43	0.53
4:D:233:ASN:O	4:D:237:ARG:HB2	2.07	0.53
2:B:184:ILE:HG12	2:B:271:ILE:HD11	1.90	0.53
4:D:205:PRO:HD3	4:D:216:VAL:HG22	1.90	0.53
7:G:64:ILE:HG22	7:G:64:ILE:O	2.08	0.53
7:G:86:PHE:HE2	7:G:90:ASP:O	1.92	0.53
3:C:252:PHE:HA	3:C:258:LEU:HD23	1.89	0.52
1:A:349:LEU:O	1:A:353:LEU:HB2	2.09	0.52
4:D:45:ILE:HA	4:D:56:MET:O	2.10	0.52
1:A:87:ASP:CG	4:D:264:THR:HG22	2.30	0.52
2:B:278:VAL:HG13	2:B:279:ALA:N	2.24	0.52
3:C:247:LEU:HA	3:C:262:GLY:HA3	1.92	0.52
5:E:14:LYS:HE2	5:E:14:LYS:CA	2.40	0.52
2:B:229:GLN:HE21	6:F:40:VAL:CB	2.22	0.52
2:B:161:ASP:HB3	2:B:187:ARG:HG3	1.92	0.52
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.45	0.52
4:D:68:GLN:NE2	4:D:73:ASP:OD2	2.31	0.52
1:A:340:LYS:HE3	1:A:344:ASP:OD2	2.09	0.52
5:E:153:ASN:C	5:E:155:LYS:H	2.12	0.52
5:E:150:ASP:OD1	5:E:151:PRO:HD2	2.10	0.51
5:E:56:LYS:HG3	5:E:170:ASN:HD21	1.75	0.51
3:C:72:THR:HA	3:C:98:ALA:CB	2.41	0.51
4:D:137:GLU:CD	4:D:158:LYS:HE2	2.30	0.51
5:E:74:TYR:O	5:E:77:GLU:HB2	2.10	0.51
3:C:107:ASN:HD22	3:C:107:ASN:C	2.12	0.51
6:F:53:ILE:N	6:F:53:ILE:HD12	2.25	0.51
5:E:18:ASN:ND2	5:E:66:ARG:NE	2.58	0.51
5:E:87:SER:HA	5:E:153:ASN:HD21	1.73	0.51
1:A:53:LYS:O	1:A:56:ASP:OD2	2.29	0.51
2:B:291:ILE:HG13	2:B:294:ARG:NH1	2.26	0.51
5:E:135:GLN:O	5:E:138:GLN:HB2	2.11	0.51
7:G:149:LYS:HB2	7:G:149:LYS:NZ	2.25	0.51
4:D:63:PHE:CD2	4:D:146:TYR:HA	2.46	0.51
2:B:180:ARG:HD2	2:B:285:THR:OG1	2.11	0.51
4:D:199:LEU:HB2	4:D:224:THR:HB	1.92	0.51
7:G:87:LYS:N	7:G:87:LYS:CE	2.73	0.51
2:B:231:GLN:HE21	2:B:231:GLN:HA	1.75	0.50
5:E:88:LYS:H	5:E:153:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ARG:HG3	2:B:180:ARG:HH11	1.76	0.50
3:C:173:ILE:O	3:C:177:GLU:HG2	2.12	0.50
4:D:188:GLY:HA3	6:F:165:LEU:HD23	1.92	0.50
2:B:286:ILE:O	2:B:294:ARG:HD3	2.12	0.50
5:E:40:ASP:OD2	5:E:143:ARG:NH2	2.34	0.50
5:E:112:PRO:O	5:E:113:LEU:HB2	2.11	0.50
6:F:91:MET:O	6:F:95:MET:HG3	2.11	0.50
2:B:225:TYR:CZ	2:B:319:ARG:HD2	2.46	0.50
3:C:14:HIS:HA	3:C:24:ALA:O	2.12	0.50
7:G:93:LYS:NZ	7:G:93:LYS:HB3	2.26	0.50
1:A:202:TYR:O	1:A:205:GLN:HB3	2.12	0.50
3:C:144:THR:N	6:F:28:GLN:NE2	2.60	0.50
5:E:14:LYS:HB2	5:E:21:LEU:HB3	1.94	0.50
5:E:32:ALA:HB2	5:E:135:GLN:OE1	2.11	0.50
6:F:80:ASP:OD1	6:F:82:ILE:HG22	2.11	0.50
1:A:185:VAL:HG11	1:A:190:ILE:HD11	1.94	0.50
1:A:372:MET:HE2	1:A:379:PHE:CD1	2.47	0.50
3:C:14:HIS:H	3:C:331:GLN:NE2	2.08	0.50
4:D:41:VAL:HG21	4:D:117:LYS:HE2	1.93	0.50
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.76	0.49
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.95	0.49
5:E:22:LEU:O	5:E:24:ILE:HG23	2.13	0.49
2:B:165:HIS:NE2	2:B:181:ARG:NE	2.60	0.49
5:E:88:LYS:H	5:E:153:ASN:HD21	1.60	0.49
1:A:400:TYR:CE1	1:A:405:PRO:HB3	2.47	0.49
2:B:339:LYS:O	2:B:340:PHE:HB3	2.13	0.49
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.47	0.49
7:G:87:LYS:N	7:G:87:LYS:HD3	2.27	0.49
2:B:239:VAL:HG23	2:B:240:LEU:CD1	2.42	0.49
2:B:291:ILE:HA	2:B:294:ARG:CG	2.43	0.49
4:D:263:HIS:HD2	4:D:266:MET:CE	2.26	0.49
1:A:237:ASP:OD2	1:A:240:LYS:HG3	2.13	0.49
4:D:75:LEU:HD23	4:D:75:LEU:O	2.12	0.49
4:D:193:HIS:CD2	4:D:194:THR:HG23	2.48	0.49
1:A:347:LEU:HD21	1:A:363:ILE:HG23	1.95	0.49
3:C:96:ASN:O	3:C:97:ARG:HD3	2.12	0.49
5:E:16:ILE:HD11	5:E:129:MET:HB2	1.94	0.49
1:A:149:LEU:HD11	1:A:180:VAL:HB	1.95	0.49
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.43	0.49
4:D:134:GLU:C	4:D:136:LYS:H	2.15	0.49
5:E:85:CYS:HB2	5:E:90:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:134:GLN:O	5:E:138:GLN:HG2	2.13	0.49
1:A:363:ILE:HD13	1:A:363:ILE:N	2.15	0.49
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.11	0.49
5:E:18:ASN:O	5:E:63:GLU:HB3	2.12	0.49
3:C:69:THR:O	3:C:76:ALA:HA	2.13	0.48
3:C:203:GLY:HA2	8:C:373:HOH:O	2.11	0.48
5:E:24:ILE:HD12	5:E:26:SER:HB2	1.95	0.48
5:E:105:ILE:HD13	5:E:130:ARG:NH1	2.27	0.48
7:G:66:THR:HB	7:G:71:VAL:HG11	1.94	0.48
1:A:204:ILE:HD12	1:A:228:LYS:HB2	1.95	0.48
3:C:74:ARG:NH1	6:F:31:GLU:HG3	2.28	0.48
5:E:84:LYS:O	5:E:85:CYS:CB	2.62	0.48
7:G:68:SER:O	7:G:71:VAL:HG13	2.13	0.48
3:C:74:ARG:HH11	6:F:31:GLU:HG3	1.77	0.48
2:B:229:GLN:NE2	6:F:40:VAL:CG1	2.73	0.48
7:G:23:LYS:CG	7:G:24:PHE:H	2.22	0.48
2:B:291:ILE:C	2:B:293:THR:N	2.66	0.48
3:C:84:ARG:O	3:C:84:ARG:HG2	2.14	0.48
4:D:65:LYS:NZ	4:D:65:LYS:CA	2.72	0.48
1:A:37:ILE:C	1:A:37:ILE:HD12	2.34	0.48
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.54	0.48
2:B:314:PRO:O	2:B:318:GLU:HG3	2.14	0.47
3:C:3:TYR:HB2	3:C:324:LEU:HG	1.95	0.47
3:C:367:LYS:NZ	3:C:368:ASP:HB3	2.28	0.47
5:E:42:VAL:HG13	5:E:140:THR:OG1	2.13	0.47
5:E:42:VAL:O	5:E:46:ILE:HG13	2.14	0.47
3:C:131:TRP:CE3	3:C:131:TRP:O	2.67	0.47
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.49	0.47
5:E:100:ILE:HA	5:E:134:GLN:HE21	1.79	0.47
2:B:184:ILE:HD11	2:B:268:PRO:HB3	1.96	0.47
2:B:291:ILE:CG2	2:B:292:ASP:H	2.16	0.47
6:F:25:PHE:CD1	6:F:67:ILE:HD13	2.50	0.47
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.96	0.47
4:D:237:ARG:O	4:D:241:ILE:HG13	2.15	0.47
1:A:129:ILE:O	1:A:133:SER:HB2	2.15	0.47
3:C:119:VAL:HG23	3:C:137:ILE:O	2.14	0.47
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.49	0.47
1:A:289:ASN:C	1:A:289:ASN:HD22	2.17	0.47
5:E:16:ILE:HG23	5:E:16:ILE:O	2.13	0.47
1:A:309:ILE:HG23	1:A:310:ASP:N	2.30	0.47
1:A:308:PRO:O	1:A:311:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:VAL:HG22	2:B:164:THR:H	1.78	0.47
1:A:343:VAL:HG23	1:A:346:ARG:NH2	2.30	0.47
2:B:302:VAL:HG13	2:B:302:VAL:O	2.14	0.47
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.49	0.47
1:A:369:THR:HA	1:A:373:GLN:OE1	2.15	0.47
4:D:223:ILE:HD12	4:D:223:ILE:N	2.30	0.47
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.50	0.46
6:F:85:ILE:HD12	6:F:86:LEU:N	2.30	0.46
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.98	0.46
3:C:371:ILE:C	3:C:372:VAL:HG23	2.36	0.46
1:A:28:GLN:HG2	4:D:10:ILE:HD13	1.95	0.46
3:C:16:TRP:CZ2	3:C:23:ILE:HD12	2.51	0.46
4:D:189:ARG:NH2	4:D:197:GLN:NE2	2.63	0.46
7:G:87:LYS:C	7:G:89:ASN:N	2.68	0.46
2:B:192:TYR:CD2	2:B:261:ALA:HA	2.50	0.46
3:C:110:LYS:HB2	3:C:123:CYS:O	2.16	0.46
5:E:58:TYR:CD2	5:E:69:ILE:HD11	2.50	0.46
5:E:153:ASN:C	5:E:155:LYS:N	2.68	0.46
1:A:174:VAL:CG1	1:A:175:THR:N	2.79	0.46
3:C:74:ARG:HH11	6:F:31:GLU:CG	2.28	0.46
1:A:106:GLU:HG2	1:A:135:ASN:HB2	1.98	0.46
5:E:70:TYR:CE2	5:E:133:LEU:HG	2.51	0.46
1:A:38:LYS:HD2	1:A:59:ASP:OD1	2.16	0.45
1:A:395:HIS:CE1	1:A:410:HIS:O	2.69	0.45
2:B:329:VAL:HG12	2:B:329:VAL:O	2.16	0.45
3:C:26:CYS:SG	3:C:55:VAL:HB	2.56	0.45
7:G:74:ARG:O	7:G:78:ILE:HG13	2.15	0.45
3:C:365:ALA:C	3:C:366:LEU:HD12	2.36	0.45
5:E:18:ASN:CG	5:E:118:ALA:H	2.19	0.45
6:F:20:LEU:O	6:F:128:LYS:HD2	2.16	0.45
1:A:397:LYS:O	1:A:401:GLU:HG3	2.16	0.45
3:C:102:VAL:HA	3:C:112:ALA:O	2.17	0.45
3:C:178:GLU:O	3:C:179:ARG:C	2.55	0.45
5:E:87:SER:OG	5:E:90:GLN:HB2	2.17	0.45
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.51	0.45
6:F:101:PHE:O	6:F:102:PHE:CD1	2.70	0.45
2:B:175:LEU:HD11	2:B:178:LEU:HD12	1.97	0.45
3:C:119:VAL:HG21	3:C:136:HIS:HB3	1.99	0.45
7:G:51:MET:HG3	7:G:87:LYS:HZ1	1.80	0.45
1:A:345:ALA:O	1:A:349:LEU:HD13	2.16	0.45
6:F:97:ARG:HB3	6:F:100:ASN:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:PHE:CD1	7:G:12:ARG:HG3	2.51	0.45
5:E:152:GLN:O	5:E:155:LYS:HD2	2.17	0.45
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.47	0.45
1:A:176:HIS:NE2	1:A:192:HIS:CE1	2.85	0.45
1:A:294:GLN:HA	1:A:295:PRO:HD3	1.85	0.45
2:B:291:ILE:HA	2:B:294:ARG:HG3	1.99	0.45
1:A:211:ARG:HD2	5:E:159:TRP:HZ3	1.82	0.45
3:C:21:THR:HG22	3:C:22:GLN:HG3	1.99	0.45
6:F:5:LEU:O	6:F:8:TYR:HB3	2.16	0.45
1:A:174:VAL:HG13	1:A:193:ILE:O	2.17	0.45
3:C:93:LEU:HB2	3:C:95:ILE:HG12	1.99	0.45
1:A:211:ARG:NH1	5:E:159:TRP:CZ3	2.86	0.44
3:C:16:TRP:CE2	3:C:335:LEU:HD21	2.51	0.44
3:C:324:LEU:O	3:C:326:LYS:HE2	2.17	0.44
7:G:87:LYS:H	7:G:87:LYS:CE	2.13	0.44
7:G:83:LEU:O	7:G:86:PHE:HB2	2.17	0.44
3:C:240:LEU:HD23	3:C:270:PHE:CD2	2.52	0.44
4:D:71:GLY:C	4:D:123:SER:OG	2.55	0.44
5:E:31:PRO:HG2	5:E:132:TYR:HB2	1.98	0.44
6:F:20:LEU:HD12	6:F:132:VAL:CG2	2.48	0.44
3:C:266:PHE:CD1	3:C:284:ARG:HG3	2.52	0.44
3:C:266:PHE:HB2	3:C:286:ASP:HB3	1.99	0.44
5:E:154:ASP:O	5:E:154:ASP:OD1	2.35	0.44
3:C:7:LEU:N	3:C:7:LEU:HD23	2.33	0.44
6:F:15:THR:CG2	6:F:63:ILE:HD12	2.47	0.44
6:F:161:ALA:O	6:F:165:LEU:HB2	2.18	0.44
7:G:113:GLY:HA3	7:G:125:LEU:HD11	1.99	0.44
1:A:389:GLU:O	1:A:393:VAL:HG22	2.17	0.44
2:B:254:VAL:HG12	2:B:258:ARG:HG3	1.99	0.44
2:B:291:ILE:C	2:B:293:THR:H	2.21	0.44
6:F:137:HIS:CE1	6:F:141:GLU:HG3	2.53	0.44
2:B:326:LEU:O	2:B:326:LEU:HG	2.16	0.44
4:D:135:GLY:O	4:D:137:GLU:HG3	2.17	0.44
6:F:76:VAL:HG12	6:F:77:LYS:N	2.33	0.44
2:B:175:LEU:HB2	2:B:177:HIS:NE2	2.32	0.43
4:D:123:SER:HB2	8:D:305:HOH:O	2.17	0.43
1:A:239:VAL:HG22	5:E:4:TYR:CZ	2.53	0.43
2:B:279:ALA:HB3	2:B:320:GLU:HG2	1.99	0.43
3:C:219:TRP:CE2	3:C:227:CYS:HB2	2.53	0.43
3:C:284:ARG:HG2	3:C:286:ASP:H	1.83	0.43
4:D:197:GLN:HG2	4:D:199:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:ASP:CG	5:E:143:ARG:HH12	2.22	0.43
7:G:11:PHE:O	7:G:14:VAL:HG12	2.17	0.43
1:A:143:VAL:HG13	1:A:146:VAL:CG2	2.48	0.43
4:D:64:TYR:HB3	4:D:92:ASN:ND2	2.32	0.43
4:D:65:LYS:NZ	4:D:68:GLN:OE1	2.52	0.43
1:A:191:LYS:HE2	1:A:303:VAL:HG22	2.01	0.43
1:A:341:ARG:O	1:A:343:VAL:N	2.52	0.43
3:C:107:ASN:ND2	3:C:107:ASN:C	2.70	0.43
4:D:247:PHE:O	4:D:250:TYR:HB3	2.18	0.43
7:G:84:ILE:C	7:G:86:PHE:H	2.20	0.43
1:A:343:VAL:O	1:A:347:LEU:HD13	2.18	0.43
4:D:184:GLU:OE1	6:F:158:ARG:HB2	2.18	0.43
4:D:265:ARG:NH1	6:F:145:GLU:OE2	2.50	0.43
1:A:343:VAL:HG21	1:A:363:ILE:HG13	1.99	0.43
4:D:189:ARG:C	4:D:191:ALA:H	2.22	0.43
5:E:22:LEU:CD2	5:E:41:ILE:HD13	2.48	0.43
7:G:68:SER:O	7:G:71:VAL:CG1	2.67	0.43
2:B:175:LEU:HD12	2:B:178:LEU:HD12	2.00	0.43
2:B:330:LEU:HB2	2:B:331:LYS:H	1.59	0.43
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.49	0.43
7:G:83:LEU:HD22	7:G:128:TRP:CE3	2.54	0.43
1:A:249:GLY:O	1:A:253:ILE:HG12	2.19	0.43
1:A:262:ILE:C	1:A:264:LYS:H	2.22	0.43
4:D:197:GLN:HG2	4:D:199:LEU:HD12	2.00	0.43
4:D:17:LEU:HD11	4:D:21:ASN:HD21	1.84	0.43
6:F:163:GLU:HA	6:F:166:LYS:CE	2.43	0.43
4:D:188:GLY:HA3	6:F:165:LEU:CD2	2.48	0.43
5:E:25:ARG:CG	5:E:35:GLU:HB3	2.34	0.43
5:E:32:ALA:CB	5:E:135:GLN:OE1	2.67	0.43
1:A:71:THR:HG23	1:A:72:TYR:CE1	2.54	0.42
1:A:111:LEU:HD23	1:A:111:LEU:C	2.39	0.42
1:A:313:ARG:HB2	1:A:314:PRO:HD3	2.00	0.42
4:D:205:PRO:CD	4:D:216:VAL:HG22	2.49	0.42
5:E:67:THR:O	5:E:71:ILE:HG13	2.19	0.42
5:E:99:GLY:O	5:E:134:GLN:HG3	2.19	0.42
5:E:106:PRO:HB3	5:E:117:TYR:HB3	2.00	0.42
7:G:23:LYS:CG	7:G:24:PHE:N	2.77	0.42
1:A:289:ASN:HD22	1:A:290:PRO:N	2.17	0.42
1:A:329:ARG:O	1:A:330:ASP:HB2	2.18	0.42
4:D:248:ARG:HD3	4:D:248:ARG:C	2.39	0.42
5:E:87:SER:HA	5:E:153:ASN:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD23	2:B:321:LEU:HD11	2.01	0.42
2:B:335:GLU:HB2	2:B:338:SER:OG	2.18	0.42
5:E:74:TYR:O	5:E:77:GLU:N	2.52	0.42
5:E:150:ASP:C	5:E:152:GLN:N	2.73	0.42
1:A:239:VAL:HG23	1:A:240:LYS:N	2.34	0.42
1:A:279:PRO:O	1:A:282:PHE:HB2	2.20	0.42
1:A:302:GLU:O	1:A:306:ASN:ND2	2.53	0.42
5:E:146:GLU:O	5:E:146:GLU:CG	2.64	0.42
6:F:73:SER:HB3	6:F:112:TYR:CG	2.55	0.42
6:F:104:LEU:HD23	6:F:104:LEU:HA	1.85	0.42
3:C:210:PHE:O	3:C:339:LYS:HD3	2.20	0.42
6:F:4:THR:C	6:F:7:PRO:HD2	2.39	0.42
7:G:124:VAL:O	7:G:127:GLN:HB2	2.20	0.42
3:C:131:TRP:O	3:C:131:TRP:HE3	2.03	0.42
3:C:244:THR:HB	3:C:264:ASP:OD2	2.19	0.42
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.81	0.42
1:A:78:ILE:C	1:A:79:ARG:HD2	2.39	0.42
3:C:209:CYS:SG	3:C:251:THR:HA	2.60	0.42
1:A:239:VAL:HG23	1:A:240:LYS:H	1.83	0.42
2:B:202:TYR:CZ	2:B:252:ILE:HB	2.54	0.42
6:F:45:GLU:OE2	6:F:45:GLU:N	2.50	0.42
1:A:272:GLY:O	1:A:274:GLU:N	2.53	0.42
3:C:144:THR:H	6:F:28:GLN:HE22	1.66	0.42
4:D:75:LEU:HD23	4:D:75:LEU:C	2.40	0.42
3:C:76:ALA:HB2	3:C:93:LEU:HD11	2.02	0.41
3:C:73:ASP:O	3:C:74:ARG:HB2	2.20	0.41
3:C:144:THR:OG1	6:F:28:GLN:NE2	2.52	0.41
1:A:55:VAL:HG23	6:F:159:ILE:HD12	2.02	0.41
1:A:190:ILE:HG22	1:A:191:LYS:N	2.34	0.41
1:A:349:LEU:HD12	1:A:349:LEU:N	2.35	0.41
3:C:188:LYS:HD3	3:C:188:LYS:HA	1.90	0.41
5:E:28:PHE:CE2	5:E:138:GLN:HB3	2.55	0.41
3:C:185:TRP:CZ2	3:C:231:ALA:HB2	2.55	0.41
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.56	0.41
4:D:129:PHE:CD2	4:D:237:ARG:HG3	2.50	0.41
5:E:82:LEU:HD11	5:E:95:MET:SD	2.61	0.41
7:G:64:ILE:O	7:G:64:ILE:CG2	2.67	0.41
7:G:75:ALA:O	7:G:79:VAL:HG23	2.20	0.41
3:C:119:VAL:HG22	3:C:120:ILE:N	2.36	0.41
4:D:53:THR:C	4:D:54:LYS:HD2	2.41	0.41
6:F:43:SER:HB2	6:F:46:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.91	0.41
1:A:176:HIS:CD2	1:A:192:HIS:NE2	2.88	0.41
3:C:257:SER:OG	3:C:372:VAL:HA	2.21	0.41
1:A:216:PRO:HB2	1:A:219:GLN:HB2	2.03	0.41
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.56	0.41
3:C:151:HIS:HB2	3:C:156:LEU:HB2	2.03	0.41
7:G:44:SER:OG	7:G:48:GLN:NE2	2.54	0.41
7:G:83:LEU:HD22	7:G:128:TRP:CE2	2.56	0.41
1:A:116:PRO:O	1:A:117:LEU:HB2	2.21	0.41
2:B:290:ASP:C	2:B:291:ILE:HD12	2.40	0.41
2:B:291:ILE:HA	2:B:294:ARG:HG2	2.03	0.41
2:B:334:VAL:O	2:B:336:LYS:N	2.54	0.41
3:C:264:ASP:O	3:C:265:CYS:HB2	2.21	0.41
2:B:291:ILE:O	2:B:293:THR:N	2.53	0.41
2:B:326:LEU:HA	2:B:330:LEU:CD1	2.51	0.41
3:C:151:HIS:CG	3:C:152:PRO:HD2	2.56	0.41
4:D:134:GLU:O	4:D:136:LYS:N	2.54	0.41
5:E:80:LYS:HA	5:E:164:VAL:HG23	2.03	0.41
2:B:280:GLU:HA	2:B:324:LEU:CD1	2.50	0.40
4:D:186:LYS:HE3	4:D:198:VAL:O	2.21	0.40
5:E:38:ASP:OD2	5:E:38:ASP:N	2.54	0.40
5:E:165:LYS:HB3	5:E:165:LYS:HE2	1.92	0.40
7:G:66:THR:HG21	7:G:71:VAL:CG2	2.47	0.40
3:C:116:GLY:C	3:C:118:ARG:H	2.25	0.40
3:C:201:SER:O	7:G:148:ARG:CG	2.69	0.40
4:D:3:LEU:HD23	4:D:250:TYR:CE1	2.57	0.40
4:D:91:TYR:CD1	4:D:91:TYR:N	2.88	0.40
4:D:132:GLN:HB2	4:D:156:SER:OG	2.22	0.40
7:G:77:SER:HA	7:G:80:LEU:HB3	2.03	0.40
7:G:120:ASN:O	7:G:123:ALA:N	2.55	0.40
1:A:71:THR:HG23	1:A:72:TYR:CD1	2.56	0.40
5:E:145:CYS:C	5:E:147:LYS:H	2.24	0.40
1:A:347:LEU:HD22	1:A:363:ILE:CD1	2.48	0.40
5:E:60:ILE:N	5:E:60:ILE:HD12	2.36	0.40
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.73	0.40
1:A:128:GLU:O	1:A:132:GLU:HB2	2.22	0.40
5:E:35:GLU:OE1	5:E:36:THR:N	2.51	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	391/418 (94%)	356 (91%)	29 (7%)	6 (2%)	10 15
2	B	197/394 (50%)	159 (81%)	29 (15%)	9 (5%)	2 2
3	C	337/372 (91%)	319 (95%)	16 (5%)	2 (1%)	25 37
4	D	273/300 (91%)	253 (93%)	18 (7%)	2 (1%)	22 33
5	E	171/178 (96%)	149 (87%)	19 (11%)	3 (2%)	8 12
6	F	164/168 (98%)	156 (95%)	7 (4%)	1 (1%)	25 37
7	G	133/151 (88%)	120 (90%)	11 (8%)	2 (2%)	10 15
All	All	1666/1981 (84%)	1512 (91%)	129 (8%)	25 (2%)	10 15

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	TYR
2	B	174	SER
2	B	278	VAL
2	B	291	ILE
2	B	331	LYS
2	B	335	GLU
4	D	202	HIS
5	E	85	CYS
5	E	153	ASN
7	G	88	ALA
6	F	102	PHE
1	A	70	PRO
2	B	171	GLU
2	B	340	PHE
1	A	264	LYS
1	A	342	THR
2	B	330	LEU
5	E	151	PRO

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Mol	Chain	Res	Type
7	G	119	ASP
1	A	310	ASP
2	B	334	VAL
3	C	179	ARG
4	D	135	GLY
1	A	262	ILE
3	C	203	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	346/363 (95%)	331 (96%)	15 (4%)	29	44
2	B	154/345 (45%)	139 (90%)	15 (10%)	8	11
3	C	290/313 (93%)	281 (97%)	9 (3%)	40	57
4	D	243/264 (92%)	233 (96%)	10 (4%)	30	46
5	E	155/159 (98%)	145 (94%)	10 (6%)	17	26
6	F	152/155 (98%)	149 (98%)	3 (2%)	55	73
7	G	108/124 (87%)	102 (94%)	6 (6%)	21	33
All	All	1448/1723 (84%)	1380 (95%)	68 (5%)	26	40

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	117	LEU
1	A	143	VAL
1	A	154	THR
1	A	191	LYS
1	A	230	ARG
1	A	243	ASN
1	A	255	GLN
1	A	282	PHE

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Mol	Chain	Res	Type
1	A	289	ASN
1	A	335	LEU
1	A	340	LYS
1	A	343	VAL
1	A	363	ILE
2	B	161	ASP
2	B	167	CYS
2	B	175	LEU
2	B	182	LEU
2	B	200	ARG
2	B	220	LEU
2	B	231	GLN
2	B	240	LEU
2	B	274	GLU
2	B	294	ARG
2	B	298	TYR
2	B	303	LEU
2	B	320	GLU
2	B	326	LEU
2	B	330	LEU
3	C	21	THR
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	210	PHE
3	C	321	LEU
3	C	367	LYS
3	C	370	LYS
4	D	6	VAL
4	D	35	PHE
4	D	65	LYS
4	D	107	ASP
4	D	116	LEU
4	D	160	ARG
4	D	171	ASP
4	D	186	LYS
4	D	230	ARG
4	D	248	ARG
5	E	22	LEU
5	E	24	ILE
5	E	63	GLU

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Mol	Chain	Res	Type
5	E	82	LEU
5	E	95	MET
5	E	144	LEU
5	E	146	GLU
5	E	151	PRO
5	E	153	ASN
5	E	159	TRP
6	F	102	PHE
6	F	104	LEU
6	F	165	LEU
7	G	39	GLU
7	G	71	VAL
7	G	86	PHE
7	G	87	LYS
7	G	97	SER
7	G	149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	157	GLN
1	A	192	HIS
1	A	206	GLN
1	A	243	ASN
1	A	255	GLN
1	A	289	ASN
1	A	306	ASN
1	A	318	ASN
1	A	370	HIS
1	A	395	HIS
2	B	205	ASN
2	B	229	GLN
2	B	231	GLN
2	B	272	ASN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	44	GLN
3	C	65	ASN
3	C	107	ASN
3	C	331	GLN

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Mol	Chain	Res	Type
4	D	21	ASN
4	D	26	ASN
4	D	49	ASN
4	D	140	ASN
4	D	197	GLN
4	D	202	HIS
4	D	231	HIS
5	E	83	GLN
5	E	90	GLN
5	E	134	GLN
5	E	153	ASN
6	F	28	GLN
6	F	100	ASN
6	F	137	HIS
7	G	48	GLN
7	G	61	ASN
7	G	89	ASN
7	G	96	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	399/418 (95%)	0.26	23 (5%)	23	19	25, 50, 88, 106	0
2	B	201/394 (51%)	0.48	27 (13%)	3	2	33, 59, 95, 102	0
3	C	341/372 (91%)	0.04	9 (2%)	56	52	28, 41, 70, 97	0
4	D	277/300 (92%)	0.13	5 (1%)	68	65	26, 45, 74, 97	0
5	E	173/178 (97%)	0.61	24 (13%)	2	2	44, 69, 101, 111	0
6	F	166/168 (98%)	-0.16	1 (0%)	89	89	27, 41, 54, 77	0
7	G	137/151 (90%)	0.63	19 (13%)	2	2	35, 79, 99, 103	0
All	All	1694/1981 (85%)	0.25	108 (6%)	19	16	25, 49, 93, 111	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	178	LEU	6.2
3	C	127	GLN	6.0
7	G	50	ASN	5.5
5	E	154	ASP	5.5
2	B	289	ALA	5.0
7	G	46	LEU	4.6
7	G	45	CYS	4.4
2	B	172	GLY	4.3
7	G	42	VAL	4.2
1	A	51	VAL	4.2
5	E	85	CYS	4.1
1	A	157	GLN	4.1
2	B	174	SER	4.1
5	E	36	THR	3.9
3	C	367	LYS	3.7
1	A	351	GLU	3.7
2	B	290	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
5	E	156	PRO	3.7
2	B	176	PRO	3.6
1	A	352	GLU	3.6
1	A	259	ILE	3.5
2	B	340	PHE	3.4
1	A	261	ALA	3.4
5	E	89	SER	3.4
3	C	129	ASN	3.3
5	E	11	PRO	3.3
5	E	150	ASP	3.3
3	C	131	TRP	3.2
3	C	275	ALA	3.2
1	A	269	ILE	3.2
2	B	181	ARG	3.2
2	B	332	GLY	3.1
5	E	84	LYS	3.1
2	B	334	VAL	3.1
7	G	13	LYS	3.1
5	E	95	MET	3.0
2	B	169	VAL	3.0
1	A	158	VAL	3.0
7	G	35	ALA	3.0
2	B	335	GLU	2.9
5	E	38	ASP	2.9
7	G	84	ILE	2.9
1	A	348	LYS	2.9
1	A	268	SER	2.9
2	B	182	LEU	2.8
6	F	4	THR	2.8
5	E	146	GLU	2.8
1	A	262	ILE	2.8
5	E	155	LYS	2.8
5	E	149	PHE	2.7
5	E	92	GLU	2.7
1	A	161	ARG	2.7
1	A	53	LYS	2.7
5	E	142	LEU	2.7
2	B	170	TYR	2.7
5	E	151	PRO	2.7
1	A	416	VAL	2.6
3	C	130	ASP	2.6
1	A	218	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
7	G	10	ARG	2.6
7	G	88	ALA	2.6
5	E	10	ASP	2.6
1	A	70	PRO	2.6
4	D	203	ARG	2.6
2	B	177	HIS	2.6
1	A	266	GLU	2.6
3	C	82	LYS	2.5
2	B	286	ILE	2.5
7	G	19	TYR	2.5
3	C	234	LYS	2.5
4	D	213	ASP	2.5
5	E	83	GLN	2.5
5	E	25	ARG	2.5
1	A	39	GLU	2.5
4	D	214	ALA	2.5
2	B	288	ALA	2.4
3	C	362	LEU	2.4
2	B	333	ASP	2.4
5	E	82	LEU	2.4
5	E	153	ASN	2.4
1	A	317	LYS	2.3
7	G	27	GLU	2.3
7	G	28	ASP	2.3
2	B	183	ASP	2.3
7	G	11	PHE	2.3
4	D	215	ALA	2.3
7	G	120	ASN	2.3
1	A	97	ILE	2.3
2	B	166	ILE	2.3
1	A	219	GLN	2.3
2	B	180	ARG	2.3
7	G	14	VAL	2.2
7	G	22	ASN	2.2
2	B	173	PHE	2.2
1	A	221	LEU	2.2
5	E	14	LYS	2.2
7	G	21	GLU	2.2
7	G	64	ILE	2.2
2	B	293	THR	2.1
2	B	274	GLU	2.1
2	B	292	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	119	LYS	2.1
4	D	249	ASP	2.0
7	G	119	ASP	2.0
2	B	331	LYS	2.0
1	A	250	SER	2.0
5	E	152	GLN	2.0
2	B	171	GLU	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.