WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:54 AM GMT

PDB ID	:	3GGR
Title	:	Crystal Structure of the Human Rad9-Hus1-Rad1 complex
Authors	:	Xu, M.; Bai, L.; Hang, H.Y.; Jiang, T.
Deposited on	:	2009-03-02
Resolution	:	3.20 Å(reported)

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

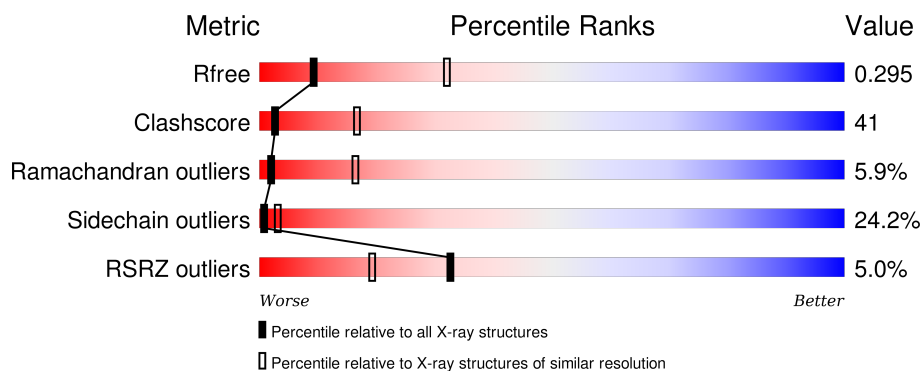|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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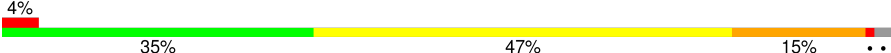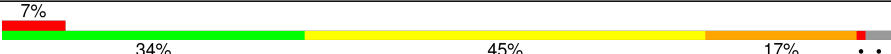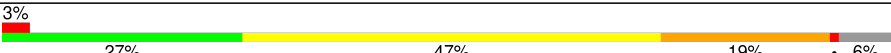*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	Percentile Ranks	Value
Rfree		0.295
Clashscore		41
Ramachandran outliers		5.9%
Sidechain outliers		24.2%
RSRZ outliers		5.0%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	270	4% 35% 47% 15% ••
2	B	286	7% 34% 45% 17% ••
3	C	282	3% 27% 47% 19% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6325 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 Cell cycle checkpoint control protein RAD9A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2038	1296	355	372	15			

- Molecule 2 is a protein called Checkpoint protein HUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	278	Total	C	N	O	S	0	0	0
			2203	1399	377	412	15			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	EXPRESSION TAG	UNP O60921
B	-4	HIS	-	EXPRESSION TAG	UNP O60921
B	-3	HIS	-	EXPRESSION TAG	UNP O60921
B	-2	HIS	-	EXPRESSION TAG	UNP O60921
B	-1	HIS	-	EXPRESSION TAG	UNP O60921
B	0	HIS	-	EXPRESSION TAG	UNP O60921
B	1	HIS	-	EXPRESSION TAG	UNP O60921

- Molecule 3 is a protein called Cell cycle checkpoint protein RAD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	264	Total	C	N	O	S	0	0	0
			2084	1320	342	404	18			

3 Residue-property plots ⓘ

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

- Molecule 1: Cell cycle checkpoint control protein RAD9A

Chain A:
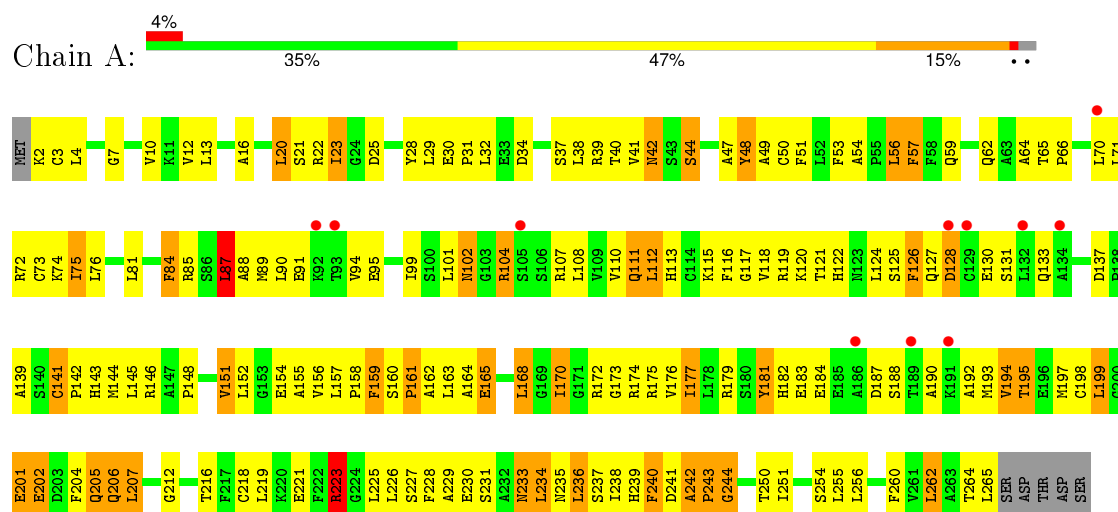
- Molecule 2: Checkpoint protein HUS1

Chain B:
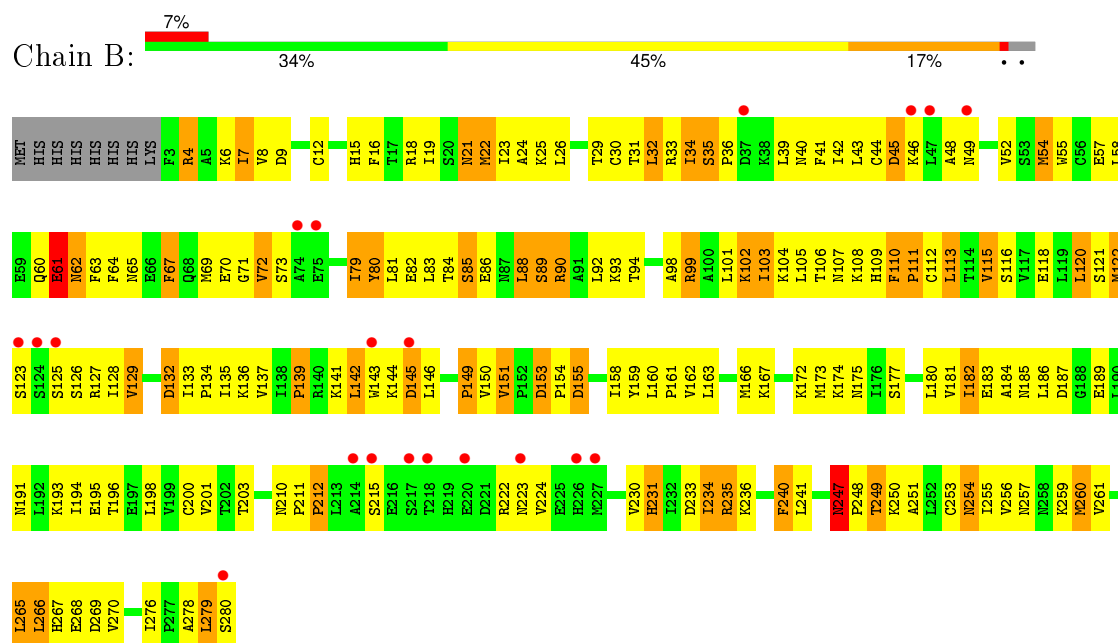
- Molecule 3: Cell cycle checkpoint protein RAD1

Chain C:

4   Data and refinement statistics (i)

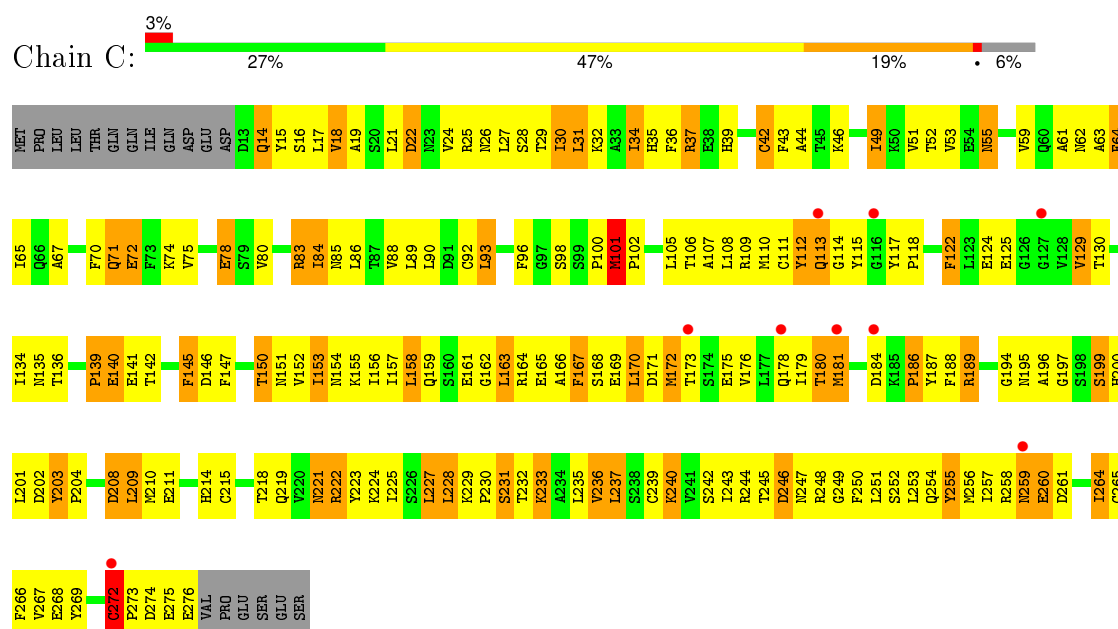| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.03Å 67.16Å 83.41Å 90.00° 97.58° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-3.20) 99.5 (15.00-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.289 , 0.306 0.286 , 0.295	Depositor DCC
R_{free} test set	1279 reflections (11.07%)	DCC
Wilson B-factor (Å^2)	84.2	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 12839 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6325	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (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	0.50	0/2075	0.80	5/2800 (0.2%)
2	B	0.52	0/2242	0.85	5/3035 (0.2%)
3	C	0.53	0/2122	0.79	2/2870 (0.1%)
All	All	0.52	0/6439	0.82	12/8705 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	MET	CB-CA-C	-5.92	98.55	110.40
2	B	153	ASP	C-N-CD	-5.84	107.75	120.60
3	C	272	CYS	N-CA-C	5.63	126.21	111.00
2	B	101	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	87	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	76	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	262	LEU	CA-CB-CG	5.23	127.33	115.30
2	B	155	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	198	LEU	CB-CA-C	5.18	120.04	110.20
1	A	73	CYS	CA-CB-SG	-5.10	104.81	114.00
2	B	125	SER	N-CA-CB	-5.09	102.87	110.50
3	C	108	LEU	CA-CB-CG	5.06	126.94	115.30

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	2038	0	2069	166	0
2	B	2203	0	2250	193	0
3	C	2084	0	2056	176	0
All	All	6325	0	6375	519	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 41.

All (519) 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)
2:B:109:HIS:O	2:B:110:PHE:CD1	1.88	1.26
2:B:79:ILE:HD12	2:B:79:ILE:C	1.53	1.24
1:A:71:LEU:O	1:A:72:ARG:HD3	1.33	1.21
2:B:110:PHE:O	2:B:110:PHE:HD1	1.25	1.17
2:B:110:PHE:O	2:B:110:PHE:CD1	1.97	1.16
3:C:153:ILE:HG22	3:C:154:ASN:H	1.01	1.16
2:B:79:ILE:O	2:B:79:ILE:HD12	1.48	1.14
1:A:71:LEU:C	1:A:72:ARG:HD3	1.66	1.13
2:B:106:THR:HG22	2:B:107:ASN:N	1.63	1.11
3:C:153:ILE:CG2	3:C:154:ASN:H	1.66	1.08
2:B:106:THR:CG2	2:B:107:ASN:H	1.62	1.08
3:C:237:LEU:HB2	3:C:258:ARG:HH22	1.18	1.07
2:B:35:SER:HB3	2:B:39:LEU:HB2	1.38	1.01
2:B:106:THR:HG22	2:B:107:ASN:H	0.86	1.00
2:B:79:ILE:C	2:B:79:ILE:CD1	2.30	0.99
2:B:113:LEU:O	2:B:134:PRO:HD2	1.61	0.99
2:B:12:CYS:HB3	2:B:63:PHE:HB2	1.44	0.99
1:A:71:LEU:O	1:A:72:ARG:CD	2.08	0.99
3:C:156:ILE:HD11	3:C:179:ILE:HD13	1.44	0.99
1:A:87:LEU:HD13	1:A:88:ALA:H	1.29	0.98
3:C:101:MET:HB2	3:C:102:PRO:HD2	1.43	0.98
2:B:55:TRP:CD1	2:B:149:PRO:HG2	2.00	0.96
3:C:153:ILE:HG22	3:C:154:ASN:N	1.79	0.95
2:B:234:ILE:HG22	2:B:235:ARG:H	1.32	0.94
1:A:254:SER:HB3	1:A:255:LEU:HD12	1.50	0.93
2:B:18:ARG:HA	2:B:21:ASN:ND2	1.84	0.92
2:B:250:LYS:HD2	2:B:266:LEU:HG	1.50	0.91
2:B:35:SER:OG	2:B:36:PRO:CD	2.20	0.90
2:B:35:SER:OG	2:B:36:PRO:HD2	1.70	0.89
3:C:113:GLN:HE21	3:C:115:TYR:HE2	1.21	0.89
1:A:146:ARG:HG3	1:A:236:LEU:HD23	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:C	1:A:75:ILE:HG12	1.94	0.87
2:B:30:CYS:HB2	2:B:42:ILE:HG23	1.57	0.85
3:C:186:PRO:O	3:C:187:TYR:CD2	2.29	0.85
3:C:24:VAL:CG1	3:C:105:LEU:HB3	2.06	0.84
2:B:69:MET:HE3	2:B:79:ILE:HG23	1.61	0.83
3:C:209:LEU:H	3:C:209:LEU:HD23	1.42	0.82
2:B:69:MET:CE	2:B:79:ILE:HG23	2.10	0.82
3:C:42:CYS:HB3	3:C:51:VAL:HG23	1.60	0.81
2:B:46:LYS:HG3	2:B:46:LYS:O	1.78	0.81
1:A:187:ASP:H	1:A:190:ALA:HB3	1.44	0.81
2:B:112:CYS:HB2	2:B:134:PRO:O	1.81	0.81
3:C:237:LEU:HB2	3:C:258:ARG:NH2	1.95	0.81
3:C:221:ASN:ND2	3:C:244:ARG:HD2	1.96	0.80
2:B:234:ILE:HD11	2:B:280:SER:OXT	1.80	0.80
3:C:236:VAL:HG13	3:C:236:VAL:O	1.82	0.80
1:A:159:PHE:HB3	1:A:195:THR:HB	1.64	0.79
3:C:178:GLN:HB3	3:C:189:ARG:HB3	1.63	0.79
3:C:158:LEU:HA	3:C:211:GLU:HG3	1.65	0.79
1:A:155:ALA:HA	1:A:197:MET:HG2	1.64	0.79
3:C:27:LEU:O	3:C:31:LEU:HB2	1.83	0.78
2:B:109:HIS:O	2:B:110:PHE:HD1	1.62	0.78
1:A:41:VAL:HG22	1:A:48:TYR:HB2	1.66	0.78
3:C:156:ILE:CD1	3:C:179:ILE:HD13	2.14	0.77
2:B:141:LYS:HG3	2:B:142:LEU:N	1.99	0.77
3:C:224:LYS:NZ	3:C:276:GLU:HG3	1.99	0.77
2:B:81:LEU:HB2	2:B:136:LYS:HD2	1.67	0.76
2:B:184:ALA:HB3	2:B:255:ILE:HD12	1.68	0.76
2:B:112:CYS:SG	2:B:133:ILE:HG23	2.25	0.76
3:C:101:MET:HB2	3:C:102:PRO:CD	2.17	0.75
1:A:193:MET:HG3	2:B:133:ILE:O	1.87	0.75
1:A:242:ALA:HB1	1:A:243:PRO:HD3	1.69	0.75
3:C:153:ILE:CG2	3:C:154:ASN:N	2.38	0.74
2:B:155:ASP:HB3	2:B:256:VAL:HA	1.69	0.74
3:C:240:LYS:HB3	3:C:256:MET:HG3	1.68	0.73
1:A:119:ARG:HB3	3:C:201:LEU:CD1	2.18	0.73
3:C:24:VAL:HG12	3:C:105:LEU:HB3	1.68	0.73
3:C:26:ASN:ND2	3:C:260:GLU:HB3	2.04	0.73
1:A:242:ALA:HB1	1:A:243:PRO:CD	2.18	0.73
2:B:64:PHE:CD2	2:B:67:PHE:HB3	2.24	0.73
3:C:224:LYS:HZ2	3:C:276:GLU:HG3	1.50	0.72
2:B:230:VAL:O	2:B:231:HIS:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ASN:CG	2:B:108:LYS:H	1.92	0.72
1:A:30:GLU:HB2	1:A:37:SER:OG	1.89	0.72
3:C:223:TYR:CZ	3:C:252:SER:HB2	2.24	0.72
1:A:99:ILE:HG13	1:A:110:VAL:HG13	1.70	0.72
2:B:71:GLY:C	2:B:73:SER:H	1.92	0.71
1:A:119:ARG:HB3	3:C:201:LEU:HD13	1.71	0.71
1:A:240:PHE:HD1	1:A:241:ASP:H	1.36	0.71
2:B:18:ARG:HA	2:B:21:ASN:HD22	1.54	0.70
1:A:65:THR:N	1:A:66:PRO:HD2	2.06	0.70
2:B:72:VAL:O	2:B:72:VAL:HG12	1.92	0.70
3:C:21:LEU:HD11	3:C:70:PHE:CD1	2.26	0.70
2:B:36:PRO:HD2	2:B:39:LEU:HD13	1.72	0.70
1:A:148:PRO:HA	1:A:234:LEU:HD12	1.74	0.70
2:B:35:SER:CB	2:B:39:LEU:HB2	2.18	0.70
2:B:79:ILE:HD12	2:B:80:TYR:N	2.04	0.70
2:B:110:PHE:HE1	2:B:112:CYS:HG	1.39	0.70
1:A:159:PHE:HB3	1:A:195:THR:CB	2.22	0.70
2:B:167:LYS:HB2	2:B:241:LEU:HG	1.73	0.69
2:B:79:ILE:O	2:B:79:ILE:CD1	2.33	0.69
2:B:19:ILE:HD11	2:B:270:VAL:HG21	1.75	0.69
2:B:240:PHE:HE1	2:B:265:LEU:HD21	1.58	0.69
2:B:4:ARG:HB3	2:B:105:LEU:HD13	1.75	0.69
3:C:227:LEU:HD11	3:C:273:PRO:HG3	1.75	0.68
3:C:274:ASP:CG	3:C:275:GLU:H	1.96	0.68
1:A:22:ARG:HG3	1:A:22:ARG:O	1.94	0.68
1:A:87:LEU:HD23	1:A:112:LEU:HG	1.76	0.68
2:B:4:ARG:O	2:B:104:LYS:HB2	1.94	0.68
2:B:48:ALA:O	2:B:49:ASN:OD1	2.11	0.68
2:B:26:LEU:HD11	2:B:54:MET:SD	2.33	0.68
2:B:110:PHE:C	2:B:110:PHE:HD1	1.97	0.68
2:B:106:THR:HG21	2:B:109:HIS:CD2	2.29	0.67
1:A:74:LYS:O	1:A:75:ILE:HG12	1.95	0.67
3:C:24:VAL:HG11	3:C:105:LEU:HB3	1.77	0.66
3:C:46:LYS:HA	3:C:75:VAL:HG11	1.77	0.66
1:A:218:CYS:SG	1:A:221:GLU:OE1	2.54	0.66
2:B:6:LYS:HE2	2:B:8:VAL:HG22	1.78	0.65
2:B:18:ARG:O	2:B:22:MET:HB2	1.95	0.65
2:B:259:LYS:CE	2:B:279:LEU:HD21	2.27	0.65
1:A:21:SER:HB2	1:A:81:LEU:HD22	1.77	0.65
3:C:228:LEU:O	3:C:231:SER:HB3	1.97	0.65
3:C:179:ILE:CD1	3:C:244:ARG:HE	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:O	1:A:233:ASN:ND2	2.30	0.65
2:B:247:ASN:OD1	2:B:247:ASN:N	2.28	0.65
2:B:35:SER:O	2:B:69:MET:HG2	1.97	0.64
1:A:117:GLY:H	3:C:204:PRO:HD2	1.62	0.64
1:A:170:ILE:HD11	1:A:172:ARG:HD2	1.78	0.64
3:C:124:GLU:HB2	3:C:129:VAL:HG13	1.79	0.64
2:B:259:LYS:HE2	2:B:279:LEU:HD21	1.79	0.64
3:C:208:ASP:HB2	3:C:211:GLU:HB3	1.80	0.64
3:C:110:MET:O	3:C:118:PRO:HD2	1.99	0.63
2:B:180:LEU:HD21	2:B:182:ILE:CD1	2.28	0.63
2:B:19:ILE:O	2:B:23:ILE:HG12	1.98	0.63
3:C:159:GLN:OE1	3:C:161:GLU:HB3	1.98	0.63
2:B:107:ASN:CG	2:B:108:LYS:N	2.52	0.62
2:B:259:LYS:HE2	2:B:279:LEU:HD11	1.80	0.62
1:A:56:LEU:HB3	1:A:255:LEU:HD23	1.81	0.62
1:A:141:CYS:HB3	1:A:240:PHE:N	2.14	0.62
2:B:201:VAL:HG13	3:C:134:ILE:HD12	1.81	0.62
2:B:234:ILE:HG22	2:B:235:ARG:N	2.11	0.62
1:A:28:TYR:HB2	1:A:39:ARG:HB3	1.80	0.62
2:B:201:VAL:HG13	3:C:134:ILE:CD1	2.30	0.62
2:B:6:LYS:HG3	2:B:7:ILE:N	2.13	0.62
3:C:34:ILE:O	3:C:53:VAL:HG21	2.00	0.62
3:C:16:SER:HB3	3:C:80:VAL:HG13	1.81	0.62
2:B:43:LEU:HD11	2:B:149:PRO:HG3	1.82	0.61
1:A:57:PHE:CZ	1:A:255:LEU:HD13	2.34	0.61
3:C:15:TYR:HD1	3:C:112:TYR:HB3	1.66	0.61
3:C:223:TYR:CE1	3:C:252:SER:HB2	2.36	0.61
1:A:71:LEU:C	1:A:72:ARG:CD	2.57	0.61
1:A:236:LEU:HB2	1:A:250:THR:OG1	2.00	0.61
1:A:156:VAL:O	1:A:160:SER:HB3	2.00	0.61
2:B:106:THR:HG21	2:B:109:HIS:NE2	2.16	0.61
3:C:53:VAL:HB	3:C:61:ALA:HB3	1.83	0.61
2:B:102:LYS:HB2	2:B:116:SER:HB3	1.81	0.61
3:C:259:ASN:HD22	3:C:259:ASN:N	1.99	0.61
3:C:244:ARG:HB2	3:C:244:ARG:NH1	2.15	0.61
2:B:180:LEU:HD21	2:B:182:ILE:HD13	1.82	0.61
2:B:141:LYS:HG3	2:B:142:LEU:H	1.65	0.61
1:A:107:ARG:HD2	1:A:125:SER:HB3	1.81	0.61
2:B:80:TYR:CZ	2:B:144:LYS:HB3	2.36	0.61
2:B:109:HIS:O	2:B:110:PHE:CE1	2.53	0.60
3:C:30:ILE:HD13	3:C:265:CYS:SG	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HD11	1:A:172:ARG:HB3	1.82	0.60
3:C:251:LEU:CB	3:C:272:CYS:HB3	2.30	0.60
2:B:71:GLY:O	2:B:73:SER:N	2.25	0.60
1:A:141:CYS:HB3	1:A:239:HIS:C	2.22	0.60
1:A:120:LYS:HE2	1:A:122:HIS:HE1	1.65	0.60
1:A:126:PHE:CG	1:A:127:GLN:N	2.67	0.60
2:B:106:THR:CG2	2:B:107:ASN:N	2.34	0.60
3:C:84:ILE:HD12	3:C:89:LEU:HD22	1.84	0.60
3:C:158:LEU:O	3:C:239:CYS:HB2	2.02	0.60
2:B:71:GLY:C	2:B:73:SER:N	2.55	0.60
1:A:161:PRO:HG3	2:B:90:ARG:HH21	1.67	0.60
3:C:275:GLU:O	3:C:276:GLU:HG2	2.02	0.60
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.15	0.59
1:A:205:GLN:NE2	1:A:234:LEU:HD11	2.18	0.59
3:C:186:PRO:O	3:C:187:TYR:HD2	1.82	0.59
3:C:246:ASP:HA	3:C:249:GLY:O	2.02	0.59
3:C:101:MET:CB	3:C:102:PRO:HD2	2.27	0.59
2:B:55:TRP:CD1	2:B:149:PRO:CG	2.83	0.59
1:A:41:VAL:CG2	1:A:48:TYR:HB2	2.33	0.59
2:B:249:THR:OG1	2:B:267:HIS:ND1	2.26	0.59
2:B:183:GLU:HG2	2:B:230:VAL:HG12	1.85	0.58
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.68	0.58
2:B:191:ASN:HA	2:B:203:THR:O	2.03	0.58
2:B:4:ARG:HH22	2:B:60:GLN:HE22	1.52	0.57
1:A:146:ARG:HG3	1:A:236:LEU:CD2	2.31	0.57
3:C:179:ILE:HD12	3:C:244:ARG:HE	1.68	0.57
3:C:112:TYR:CD2	3:C:113:GLN:N	2.72	0.57
1:A:95:GLU:HB2	1:A:113:HIS:O	2.04	0.57
1:A:193:MET:HA	2:B:135:ILE:HD11	1.85	0.57
2:B:4:ARG:HH12	2:B:67:PHE:HD1	1.53	0.57
1:A:38:LEU:O	1:A:50:CYS:HA	2.03	0.57
1:A:13:LEU:HD23	1:A:84:PHE:CZ	2.39	0.57
1:A:168:LEU:O	1:A:170:ILE:HG22	2.05	0.57
3:C:44:ALA:HB3	3:C:80:VAL:HB	1.87	0.57
3:C:92:CYS:SG	3:C:134:ILE:HG21	2.45	0.57
1:A:172:ARG:HG2	1:A:173:GLY:N	2.19	0.57
2:B:15:HIS:O	2:B:19:ILE:HG12	2.03	0.56
2:B:110:PHE:O	2:B:111:PRO:C	2.43	0.56
1:A:23:ILE:HD13	1:A:260:PHE:CE2	2.40	0.56
3:C:235:LEU:HD23	3:C:256:MET:SD	2.45	0.56
1:A:148:PRO:HA	1:A:234:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:ILE:O	3:C:264:ILE:HG12	2.05	0.56
2:B:64:PHE:HD2	2:B:67:PHE:HB3	1.69	0.56
3:C:22:ASP:H	3:C:71:GLN:HE21	1.52	0.56
2:B:121:SER:HB2	2:B:128:ILE:HG13	1.87	0.56
2:B:62:ASN:ND2	2:B:63:PHE:HD1	2.04	0.56
1:A:175:ARG:HH21	1:A:207:LEU:HD23	1.70	0.56
2:B:62:ASN:HD22	2:B:63:PHE:N	2.03	0.56
2:B:259:LYS:HD3	2:B:278:ALA:HB3	1.87	0.56
2:B:81:LEU:HA	2:B:139:PRO:HD3	1.88	0.56
3:C:21:LEU:HA	3:C:71:GLN:HG2	1.88	0.56
1:A:112:LEU:HB2	1:A:119:ARG:HG2	1.87	0.55
3:C:37:ARG:NH1	3:C:55:ASN:O	2.37	0.55
2:B:61:GLU:HG3	2:B:62:ASN:N	2.22	0.55
1:A:121:THR:HG22	3:C:199:SER:HB2	1.88	0.55
1:A:168:LEU:HD12	1:A:216:THR:OG1	2.07	0.55
3:C:253:LEU:O	3:C:253:LEU:HG	2.07	0.55
2:B:69:MET:HE1	2:B:79:ILE:HG23	1.85	0.55
2:B:24:ALA:HA	2:B:85:SER:HB3	1.86	0.55
2:B:222:ARG:HG2	2:B:223:ASN:H	1.72	0.55
1:A:42:ASN:HB2	1:A:47:ALA:H	1.72	0.55
2:B:185:ASN:HB2	2:B:189:GLU:HB3	1.89	0.55
1:A:117:GLY:N	3:C:204:PRO:HD2	2.21	0.55
3:C:89:LEU:HD11	3:C:93:LEU:HD21	1.88	0.55
1:A:4:LEU:HD22	1:A:59:GLN:HB3	1.89	0.55
3:C:171:ASP:C	3:C:172:MET:HG2	2.27	0.55
3:C:245:THR:OG1	3:C:251:LEU:HG	2.07	0.55
3:C:39:HIS:HB2	3:C:83:ARG:NH1	2.22	0.55
2:B:31:THR:N	2:B:43:LEU:O	2.37	0.55
2:B:106:THR:HG22	2:B:107:ASN:OD1	2.07	0.54
2:B:110:PHE:HE1	2:B:112:CYS:SG	2.30	0.54
1:A:160:SER:HB2	1:A:223:ARG:HH22	1.72	0.54
3:C:222:ARG:HD3	3:C:275:GLU:OE2	2.06	0.54
2:B:103:ILE:O	2:B:103:ILE:HG13	2.08	0.54
3:C:209:LEU:CD2	3:C:209:LEU:H	2.18	0.54
2:B:234:ILE:HD13	2:B:236:LYS:HE2	1.89	0.54
3:C:59:VAL:HG21	3:C:227:LEU:CB	2.38	0.54
3:C:227:LEU:CD1	3:C:273:PRO:HG3	2.38	0.54
3:C:165:GLU:O	3:C:168:SER:HB2	2.08	0.54
3:C:251:LEU:HB2	3:C:272:CYS:HB3	1.90	0.54
3:C:264:ILE:H	3:C:264:ILE:HD13	1.73	0.54
3:C:251:LEU:HB3	3:C:272:CYS:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PRO:HA	2:B:94:THR:HG21	1.89	0.54
3:C:155:LYS:HG2	3:C:214:HIS:HB2	1.90	0.54
3:C:187:TYR:HB3	3:C:202:ASP:OD1	2.08	0.54
3:C:30:ILE:HG13	3:C:258:ARG:HD2	1.90	0.53
2:B:86:GLU:O	2:B:89:SER:N	2.41	0.53
2:B:63:PHE:CD2	2:B:63:PHE:O	2.61	0.53
3:C:15:TYR:HA	3:C:112:TYR:HB3	1.91	0.53
1:A:64:ALA:C	1:A:66:PRO:HD2	2.28	0.53
2:B:106:THR:CG2	2:B:107:ASN:OD1	2.57	0.53
1:A:172:ARG:CG	1:A:173:GLY:N	2.71	0.53
1:A:160:SER:O	1:A:162:ALA:N	2.41	0.53
2:B:55:TRP:HB2	2:B:149:PRO:HB2	1.89	0.53
1:A:254:SER:CB	1:A:255:LEU:HD12	2.31	0.53
2:B:144:LYS:CG	2:B:145:ASP:N	2.72	0.53
3:C:229:LYS:HB3	3:C:230:PRO:CD	2.38	0.53
3:C:236:VAL:CG1	3:C:236:VAL:O	2.53	0.53
1:A:160:SER:HB2	1:A:223:ARG:NH2	2.24	0.52
2:B:112:CYS:SG	2:B:133:ILE:CG2	2.97	0.52
3:C:274:ASP:CG	3:C:275:GLU:N	2.61	0.52
2:B:173:MET:HB3	2:B:194:ILE:HD12	1.91	0.52
2:B:186:LEU:HG	2:B:187:ASP:OD2	2.09	0.52
1:A:148:PRO:HB2	1:A:151:VAL:HG13	1.92	0.52
1:A:154:GLU:O	1:A:158:PRO:HD3	2.09	0.52
3:C:29:THR:O	3:C:32:LYS:N	2.43	0.52
1:A:226:LEU:O	1:A:229:ALA:HB2	2.09	0.52
1:A:159:PHE:O	1:A:161:PRO:HD2	2.10	0.51
1:A:164:ALA:O	1:A:219:LEU:HB3	2.10	0.51
2:B:259:LYS:NZ	2:B:279:LEU:HD21	2.25	0.51
3:C:62:ASN:HB2	3:C:268:GLU:HB3	1.92	0.51
1:A:142:PRO:HG2	1:A:143:HIS:CD2	2.45	0.51
2:B:55:TRP:HD1	2:B:149:PRO:HG2	1.65	0.51
1:A:89:MET:HG3	1:A:90:LEU:HD12	1.92	0.51
1:A:199:LEU:CD1	2:B:128:ILE:HG23	2.40	0.51
2:B:81:LEU:HD22	2:B:136:LYS:HD2	1.92	0.51
2:B:177:SER:HB3	2:B:194:ILE:HD13	1.93	0.51
1:A:31:PRO:O	1:A:72:ARG:NH2	2.43	0.51
3:C:224:LYS:H	3:C:273:PRO:HG2	1.76	0.51
3:C:175:GLU:HB2	3:C:225:ILE:HG13	1.92	0.51
1:A:177:ILE:HG12	1:A:204:PHE:CZ	2.45	0.51
2:B:133:ILE:HG22	2:B:133:ILE:O	2.11	0.51
1:A:161:PRO:HB2	1:A:163:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:HD21	1:A:104:ARG:HE	1.59	0.51
3:C:112:TYR:HD2	3:C:113:GLN:N	2.08	0.51
3:C:257:ILE:HG22	3:C:257:ILE:O	2.10	0.51
1:A:20:LEU:O	1:A:23:ILE:HG22	2.10	0.51
3:C:52:THR:OG1	3:C:62:ASN:ND2	2.39	0.51
1:A:165:GLU:O	1:A:218:CYS:HA	2.11	0.51
3:C:36:PHE:HE2	3:C:269:TYR:HH	1.59	0.51
3:C:89:LEU:CD1	3:C:93:LEU:HD21	2.41	0.51
2:B:150:VAL:O	2:B:151:VAL:HG13	2.10	0.51
1:A:72:ARG:N	1:A:72:ARG:HD3	2.21	0.50
3:C:152:VAL:HG13	3:C:243:ILE:HG23	1.93	0.50
2:B:113:LEU:O	2:B:134:PRO:CD	2.46	0.50
1:A:119:ARG:HB3	3:C:201:LEU:HD11	1.93	0.50
1:A:160:SER:C	1:A:162:ALA:H	2.14	0.50
2:B:120:LEU:HD23	2:B:122:MET:HG2	1.93	0.50
1:A:13:LEU:HA	1:A:16:ALA:HB3	1.92	0.50
3:C:42:CYS:CB	3:C:51:VAL:HG23	2.37	0.50
2:B:180:LEU:CD2	2:B:182:ILE:HD13	2.42	0.50
2:B:185:ASN:CB	2:B:189:GLU:HB3	2.41	0.50
2:B:9:ASP:HB2	2:B:65:ASN:HD21	1.77	0.50
1:A:74:LYS:C	1:A:75:ILE:CG1	2.70	0.50
3:C:245:THR:O	3:C:250:PHE:HA	2.10	0.50
1:A:243:PRO:O	1:A:244:GLY:C	2.50	0.50
1:A:102:ASN:ND2	1:A:104:ARG:HE	2.09	0.50
2:B:19:ILE:HG21	2:B:58:LEU:HD22	1.93	0.50
2:B:4:ARG:NE	2:B:34:ILE:HG12	2.26	0.50
1:A:160:SER:CB	1:A:223:ARG:HH22	2.25	0.49
3:C:178:GLN:CB	3:C:189:ARG:HB3	2.38	0.49
1:A:187:ASP:N	1:A:190:ALA:HB3	2.22	0.49
3:C:176:VAL:HG22	3:C:222:ARG:HG3	1.94	0.49
3:C:171:ASP:O	3:C:173:THR:HG23	2.12	0.49
2:B:144:LYS:HG2	2:B:145:ASP:H	1.76	0.49
1:A:230:GLU:H	1:A:233:ASN:HD21	1.61	0.49
3:C:255:TYR:HB3	3:C:268:GLU:HG3	1.94	0.49
3:C:208:ASP:HB2	3:C:211:GLU:O	2.12	0.49
1:A:168:LEU:HD23	1:A:170:ILE:CG2	2.43	0.49
1:A:176:VAL:HG23	1:A:199:LEU:O	2.12	0.49
2:B:183:GLU:HB2	2:B:191:ASN:HB2	1.93	0.49
2:B:12:CYS:CB	2:B:63:PHE:HB2	2.30	0.49
1:A:75:ILE:CD1	1:A:108:LEU:HD22	2.43	0.49
2:B:256:VAL:HB	2:B:260:MET:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LYS:CG	2:B:145:ASP:H	2.25	0.49
1:A:182:HIS:HD2	1:A:194:VAL:HG11	1.78	0.49
3:C:152:VAL:O	3:C:244:ARG:O	2.31	0.48
3:C:203:TYR:CD2	3:C:203:TYR:N	2.80	0.48
2:B:110:PHE:CE1	2:B:112:CYS:SG	3.04	0.48
3:C:180:THR:HG23	3:C:181:MET:N	2.28	0.48
1:A:28:TYR:CE1	1:A:131:SER:HB2	2.48	0.48
1:A:228:PHE:HE2	1:A:256:LEU:HD21	1.79	0.48
3:C:59:VAL:HG21	3:C:227:LEU:HB2	1.96	0.48
3:C:175:GLU:HB3	3:C:223:TYR:HB2	1.94	0.48
3:C:152:VAL:HG12	3:C:153:ILE:O	2.13	0.48
2:B:115:VAL:HG23	2:B:132:ASP:HB2	1.95	0.48
2:B:80:TYR:OH	2:B:144:LYS:HB3	2.13	0.48
2:B:81:LEU:HD13	2:B:136:LYS:HD2	1.96	0.48
2:B:160:LEU:HD13	2:B:163:LEU:HD11	1.96	0.48
2:B:233:ASP:OD1	2:B:234:ILE:N	2.41	0.47
3:C:232:THR:O	3:C:236:VAL:HG12	2.13	0.47
2:B:181:VAL:HB	2:B:193:LYS:HB3	1.95	0.47
1:A:87:LEU:CD1	1:A:88:ALA:H	2.14	0.47
1:A:13:LEU:HD23	1:A:84:PHE:CE2	2.49	0.47
1:A:242:ALA:CB	1:A:243:PRO:CD	2.91	0.47
3:C:21:LEU:O	3:C:106:THR:OG1	2.32	0.47
2:B:248:PRO:HA	2:B:267:HIS:HB2	1.96	0.47
2:B:35:SER:OG	2:B:36:PRO:HD3	2.11	0.47
1:A:53:PHE:CE1	1:A:256:LEU:CD1	2.98	0.47
1:A:205:GLN:HE22	1:A:234:LEU:HD11	1.78	0.47
1:A:39:ARG:NH2	1:A:133:GLN:O	2.48	0.47
3:C:84:ILE:HG22	3:C:136:THR:HG22	1.95	0.47
3:C:122:PHE:C	3:C:122:PHE:CD1	2.87	0.47
2:B:55:TRP:HD1	2:B:149:PRO:CG	2.26	0.47
2:B:259:LYS:HE2	2:B:279:LEU:CD1	2.45	0.47
1:A:230:GLU:O	1:A:231:SER:HB2	2.14	0.47
1:A:152:LEU:HD22	1:A:179:ARG:HH21	1.80	0.47
1:A:117:GLY:HA2	3:C:202:ASP:O	2.15	0.47
2:B:72:VAL:CG1	2:B:72:VAL:O	2.62	0.47
3:C:117:TYR:HB3	3:C:136:THR:O	2.15	0.47
1:A:206:GLN:HB2	1:A:206:GLN:HE21	1.56	0.47
3:C:49:ILE:HD13	3:C:109:ARG:HH22	1.80	0.47
2:B:184:ALA:CB	2:B:255:ILE:HD12	2.42	0.47
2:B:181:VAL:HG11	2:B:193:LYS:NZ	2.30	0.47
3:C:150:THR:HB	3:C:247:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:HIS:C	2:B:110:PHE:CD1	2.78	0.47
1:A:87:LEU:HD22	1:A:88:ALA:N	2.30	0.47
3:C:166:ALA:HB1	3:C:201:LEU:HG	1.97	0.47
3:C:31:LEU:O	3:C:34:ILE:HG13	2.15	0.47
1:A:107:ARG:NH1	1:A:125:SER:OG	2.42	0.46
1:A:182:HIS:CG	1:A:183:GLU:N	2.83	0.46
2:B:19:ILE:CD1	2:B:270:VAL:HG21	2.42	0.46
2:B:103:ILE:HD13	2:B:113:LEU:HD11	1.97	0.46
1:A:201:GLU:HG3	1:A:202:GLU:H	1.81	0.46
3:C:24:VAL:HG12	3:C:105:LEU:CB	2.42	0.46
2:B:136:LYS:HG2	2:B:137:VAL:N	2.31	0.46
2:B:6:LYS:NZ	2:B:60:GLN:HG2	2.31	0.46
1:A:111:GLN:HB3	1:A:120:LYS:HG3	1.98	0.46
3:C:59:VAL:HG21	3:C:227:LEU:HB3	1.98	0.46
2:B:256:VAL:HB	2:B:260:MET:HB3	1.98	0.46
3:C:21:LEU:HD11	3:C:70:PHE:HD1	1.75	0.46
2:B:153:ASP:N	2:B:153:ASP:OD1	2.48	0.46
2:B:35:SER:HB3	2:B:39:LEU:CB	2.28	0.46
1:A:225:LEU:CD2	1:A:235:ASN:HD21	2.29	0.46
2:B:23:ILE:HG13	2:B:42:ILE:HD13	1.98	0.46
3:C:235:LEU:CD2	3:C:267:VAL:CG2	2.94	0.46
3:C:21:LEU:N	3:C:107:ALA:O	2.34	0.46
1:A:145:LEU:HB3	1:A:237:SER:HB2	1.98	0.46
3:C:83:ARG:HB3	3:C:139:PRO:HG2	1.97	0.46
1:A:7:GLY:O	1:A:10:VAL:HB	2.16	0.46
1:A:126:PHE:CD2	1:A:127:GLN:N	2.85	0.45
3:C:155:LYS:CG	3:C:214:HIS:HB2	2.46	0.45
1:A:54:ALA:HB3	1:A:255:LEU:HB3	1.97	0.45
3:C:145:PHE:CD2	3:C:147:PHE:HE2	2.34	0.45
2:B:12:CYS:O	2:B:16:PHE:N	2.46	0.45
2:B:55:TRP:CZ2	2:B:57:GLU:HB2	2.52	0.45
1:A:51:PHE:HE2	1:A:260:PHE:CE1	2.34	0.45
3:C:19:ALA:HA	3:C:72:GLU:O	2.17	0.45
2:B:30:CYS:CB	2:B:42:ILE:HG23	2.37	0.45
3:C:46:LYS:HG3	3:C:78:GLU:OE1	2.15	0.45
3:C:199:SER:C	3:C:200:HIS:HD2	2.20	0.45
2:B:234:ILE:CG2	2:B:235:ARG:H	2.12	0.45
3:C:167:PHE:O	3:C:167:PHE:CG	2.69	0.45
2:B:211:PRO:HA	2:B:212:PRO:HD3	1.79	0.45
1:A:172:ARG:HB2	1:A:212:GLY:HA2	1.97	0.45
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:GLU:HB2	2:B:200:CYS:SG	2.57	0.45
3:C:232:THR:O	3:C:233:LYS:C	2.55	0.45
1:A:161:PRO:O	1:A:162:ALA:HB3	2.17	0.45
3:C:67:ALA:HA	3:C:70:PHE:CD2	2.52	0.45
2:B:249:THR:HG1	2:B:267:HIS:HD1	1.55	0.45
3:C:93:LEU:HG	3:C:93:LEU:H	1.61	0.45
1:A:113:HIS:HA	1:A:118:VAL:HG22	1.97	0.45
3:C:18:VAL:HG13	3:C:74:LYS:HB3	1.99	0.45
2:B:155:ASP:CG	2:B:257:ASN:H	2.20	0.44
1:A:57:PHE:CD2	1:A:255:LEU:HB2	2.53	0.44
1:A:57:PHE:CD1	1:A:255:LEU:HD22	2.52	0.44
2:B:113:LEU:HD22	2:B:113:LEU:HA	1.76	0.44
1:A:243:PRO:HA	1:A:264:THR:HG22	2.00	0.44
3:C:235:LEU:HD22	3:C:267:VAL:CG2	2.48	0.44
3:C:157:ILE:HG21	3:C:210:MET:O	2.17	0.44
3:C:31:LEU:HB3	3:C:90:LEU:HD21	2.00	0.44
2:B:88:LEU:HD22	2:B:88:LEU:HA	1.82	0.44
3:C:35:HIS:HB2	3:C:90:LEU:HD11	2.00	0.44
3:C:221:ASN:N	3:C:221:ASN:ND2	2.65	0.44
1:A:235:ASN:C	1:A:236:LEU:HG	2.39	0.43
1:A:57:PHE:CG	1:A:255:LEU:HD22	2.53	0.43
3:C:15:TYR:CD1	3:C:112:TYR:HB3	2.49	0.43
2:B:40:ASN:HB2	2:B:60:GLN:OE1	2.18	0.43
3:C:64:PHE:N	3:C:64:PHE:CD1	2.85	0.43
3:C:244:ARG:HB2	3:C:244:ARG:CZ	2.48	0.43
2:B:55:TRP:HB2	2:B:149:PRO:CB	2.48	0.43
1:A:51:PHE:HB3	1:A:53:PHE:CE2	2.53	0.43
3:C:231:SER:HB2	3:C:269:TYR:CD1	2.54	0.43
1:A:115:LYS:HB3	1:A:116:PHE:H	1.75	0.43
2:B:155:ASP:CB	2:B:256:VAL:HA	2.41	0.43
3:C:67:ALA:HA	3:C:70:PHE:HD2	1.83	0.43
1:A:221:GLU:HB3	1:A:262:LEU:HD22	2.01	0.43
1:A:81:LEU:O	1:A:85:ARG:N	2.51	0.43
1:A:152:LEU:HD22	1:A:179:ARG:NH2	2.33	0.43
1:A:57:PHE:CE1	1:A:255:LEU:HD13	2.54	0.43
1:A:65:THR:N	1:A:66:PRO:CD	2.80	0.43
1:A:170:ILE:CD1	1:A:172:ARG:HB3	2.49	0.43
2:B:254:ASN:N	2:B:254:ASN:OD1	2.51	0.43
2:B:158:ILE:HG12	2:B:159:TYR:O	2.18	0.43
3:C:180:THR:HG22	3:C:186:PRO:HA	2.00	0.43
1:A:160:SER:C	1:A:162:ALA:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:PRO:HA	3:C:134:ILE:O	2.19	0.43
2:B:118:GLU:HG2	2:B:129:VAL:CG1	2.49	0.43
1:A:170:ILE:CG1	1:A:172:ARG:HB3	2.49	0.42
1:A:145:LEU:HA	1:A:206:GLN:O	2.19	0.42
1:A:72:ARG:HB2	1:A:130:GLU:OE1	2.19	0.42
2:B:163:LEU:HD21	2:B:251:ALA:HB1	2.01	0.42
2:B:233:ASP:CG	2:B:234:ILE:H	2.23	0.42
1:A:16:ALA:HB1	1:A:53:PHE:HZ	1.85	0.42
1:A:107:ARG:HD2	1:A:125:SER:CB	2.49	0.42
3:C:173:THR:HG21	3:C:194:GLY:CA	2.50	0.42
2:B:18:ARG:HA	2:B:21:ASN:HD21	1.75	0.42
3:C:24:VAL:HG12	3:C:105:LEU:O	2.19	0.42
1:A:143:HIS:HD2	1:A:239:HIS:O	2.02	0.42
2:B:44:CYS:O	2:B:45:ASP:HB2	2.20	0.42
2:B:180:LEU:O	2:B:233:ASP:N	2.53	0.42
3:C:83:ARG:O	3:C:139:PRO:HD2	2.19	0.42
3:C:162:GLY:O	3:C:165:GLU:HB2	2.19	0.42
1:A:88:ALA:C	1:A:90:LEU:N	2.73	0.42
1:A:12:VAL:O	1:A:16:ALA:HB2	2.20	0.42
3:C:208:ASP:HA	3:C:211:GLU:HB3	2.02	0.42
3:C:219:GLN:HE22	3:C:250:PHE:HE1	1.68	0.42
2:B:99:ARG:NE	2:B:99:ARG:HA	2.33	0.42
1:A:117:GLY:H	3:C:204:PRO:CD	2.29	0.42
1:A:157:LEU:N	1:A:158:PRO:CD	2.82	0.42
1:A:102:ASN:HD21	1:A:104:ARG:NE	2.18	0.42
2:B:63:PHE:O	2:B:63:PHE:CG	2.72	0.42
3:C:181:MET:HB2	3:C:218:THR:HB	2.01	0.42
1:A:29:LEU:HD12	1:A:38:LEU:CD2	2.50	0.42
2:B:79:ILE:CD1	2:B:80:TYR:N	2.76	0.42
3:C:178:GLN:O	3:C:188:PHE:HA	2.19	0.42
3:C:122:PHE:HA	3:C:130:THR:O	2.20	0.42
1:A:124:LEU:O	3:C:196:ALA:HB1	2.20	0.42
2:B:172:LYS:O	2:B:175:ASN:HB2	2.20	0.42
3:C:51:VAL:HG12	3:C:63:ALA:HB3	2.02	0.41
3:C:158:LEU:HD22	3:C:163:LEU:HD12	2.02	0.41
1:A:42:ASN:HD22	1:A:44:SER:CB	2.33	0.41
3:C:29:THR:HA	3:C:32:LYS:HB3	2.02	0.41
3:C:257:ILE:HG12	3:C:266:PHE:CE2	2.54	0.41
2:B:92:LEU:HD23	2:B:92:LEU:HA	1.89	0.41
2:B:19:ILE:HG21	2:B:58:LEU:CD2	2.50	0.41
1:A:240:PHE:CD1	1:A:241:ASP:N	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:THR:HG23	2:B:82:GLU:HB3	2.02	0.41
2:B:98:ALA:HB1	2:B:99:ARG:H	1.65	0.41
1:A:223:ARG:NH1	1:A:223:ARG:CG	2.79	0.41
1:A:219:LEU:O	1:A:219:LEU:HG	2.21	0.41
3:C:150:THR:HB	3:C:247:ASN:HB3	2.03	0.41
2:B:279:LEU:O	2:B:280:SER:OXT	2.39	0.41
2:B:210:ASN:HA	2:B:211:PRO:HD3	1.90	0.41
1:A:51:PHE:HE2	1:A:260:PHE:HE1	1.69	0.41
1:A:182:HIS:HD2	1:A:194:VAL:CG1	2.33	0.41
3:C:154:ASN:HD22	3:C:179:ILE:HB	1.84	0.41
3:C:188:PHE:O	3:C:202:ASP:HA	2.20	0.41
2:B:81:LEU:HB2	2:B:136:LYS:CD	2.45	0.41
2:B:259:LYS:HE2	2:B:279:LEU:CD2	2.47	0.41
3:C:75:VAL:HG23	3:C:80:VAL:HG21	2.03	0.41
3:C:179:ILE:HD12	3:C:244:ARG:NE	2.34	0.41
1:A:225:LEU:HD12	1:A:260:PHE:CD1	2.56	0.41
2:B:256:VAL:HB	2:B:260:MET:HB2	2.03	0.41
2:B:268:GLU:HG3	2:B:269:ASP:H	1.84	0.41
2:B:32:LEU:HG	2:B:33:ARG:N	2.35	0.41
1:A:181:TYR:O	1:A:182:HIS:HB2	2.21	0.41
1:A:40:THR:O	1:A:49:ALA:N	2.52	0.41
3:C:31:LEU:CD1	3:C:86:LEU:HD11	2.51	0.40
2:B:4:ARG:HD2	2:B:105:LEU:CD1	2.51	0.40
2:B:247:ASN:HA	2:B:248:PRO:HD2	1.92	0.40
3:C:251:LEU:HB3	3:C:272:CYS:HB3	1.98	0.40
1:A:227:SER:C	1:A:229:ALA:H	2.24	0.40
1:A:56:LEU:HB3	1:A:255:LEU:CD2	2.49	0.40
2:B:4:ARG:HG2	2:B:4:ARG:HH11	1.85	0.40
2:B:6:LYS:CD	2:B:60:GLN:HE21	2.34	0.40
3:C:14:GLN:HE21	3:C:14:GLN:HB2	1.63	0.40
2:B:58:LEU:HB3	2:B:270:VAL:HG12	2.03	0.40
3:C:118:PRO:HA	3:C:135:ASN:HA	2.04	0.40
3:C:62:ASN:O	3:C:267:VAL:HB	2.22	0.40
1:A:205:GLN:H	1:A:205:GLN:HG2	1.37	0.40
1:A:127:GLN:O	1:A:128:ASP:C	2.59	0.40
1:A:4:LEU:HD22	1:A:59:GLN:CB	2.52	0.40
3:C:170:LEU:HG	3:C:170:LEU:H	1.70	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	262/270 (97%)	200 (76%)	50 (19%)	12 (5%)	3	23
2	B	276/286 (96%)	207 (75%)	52 (19%)	17 (6%)	2	14
3	C	262/282 (93%)	203 (78%)	41 (16%)	18 (7%)	1	10
All	All	800/838 (96%)	610 (76%)	143 (18%)	47 (6%)	2	16

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	243	PRO
2	B	35	SER
2	B	45	ASP
2	B	72	VAL
2	B	99	ARG
3	C	101	MET
1	A	94	VAL
1	A	128	ASP
1	A	242	ALA
2	B	52	VAL
2	B	143	TRP
2	B	149	PRO
2	B	231	HIS
3	C	113	GLN
3	C	140	GLU
1	A	139	ALA
1	A	223	ARG
2	B	70	GLU
2	B	111	PRO
2	B	123	SER
3	C	78	GLU
3	C	153	ILE
3	C	231	SER

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Mol	Chain	Res	Type
3	C	233	LYS
1	A	126	PHE
1	A	188	SER
1	A	192	ALA
2	B	61	GLU
2	B	154	PRO
2	B	212	PRO
3	C	55	ASN
3	C	85	ASN
3	C	142	THR
3	C	195	ASN
3	C	272	CYS
2	B	161	PRO
2	B	235	ARG
3	C	261	ASP
1	A	244	GLY
2	B	247	ASN
3	C	100	PRO
1	A	161	PRO
3	C	186	PRO
3	C	197	GLY
3	C	114	GLY
3	C	139	PRO

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	223/229 (97%)	173 (78%)	50 (22%)	1	5
2	B	255/263 (97%)	198 (78%)	57 (22%)	1	5
3	C	238/256 (93%)	172 (72%)	66 (28%)	0	1
All	All	716/748 (96%)	543 (76%)	173 (24%)	1	3

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	CYS
1	A	20	LEU
1	A	23	ILE
1	A	25	ASP
1	A	32	LEU
1	A	34	ASP
1	A	44	SER
1	A	48	TYR
1	A	56	LEU
1	A	57	PHE
1	A	62	GLN
1	A	70	LEU
1	A	75	ILE
1	A	84	PHE
1	A	87	LEU
1	A	91	GLU
1	A	101	LEU
1	A	102	ASN
1	A	104	ARG
1	A	111	GLN
1	A	112	LEU
1	A	137	ASP
1	A	141	CYS
1	A	151	VAL
1	A	159	PHE
1	A	165	GLU
1	A	168	LEU
1	A	170	ILE
1	A	174	ARG
1	A	177	ILE
1	A	181	TYR
1	A	184	GLU
1	A	194	VAL
1	A	195	THR
1	A	198	CYS
1	A	199	LEU
1	A	201	GLU
1	A	202	GLU
1	A	205	GLN
1	A	206	GLN
1	A	207	LEU
1	A	223	ARG

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	234	LEU
1	A	236	LEU
1	A	238	ILE
1	A	240	PHE
1	A	251	ILE
1	A	265	LEU
2	B	4	ARG
2	B	7	ILE
2	B	21	ASN
2	B	22	MET
2	B	25	LYS
2	B	29	THR
2	B	32	LEU
2	B	34	ILE
2	B	41	PHE
2	B	54	MET
2	B	61	GLU
2	B	62	ASN
2	B	67	PHE
2	B	79	ILE
2	B	80	TYR
2	B	83	LEU
2	B	84	THR
2	B	85	SER
2	B	88	LEU
2	B	89	SER
2	B	90	ARG
2	B	93	LYS
2	B	102	LYS
2	B	103	ILE
2	B	110	PHE
2	B	113	LEU
2	B	115	VAL
2	B	120	LEU
2	B	122	MET
2	B	126	SER
2	B	127	ARG
2	B	129	VAL
2	B	132	ASP
2	B	139	PRO
2	B	142	LEU

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Mol	Chain	Res	Type
2	B	145	ASP
2	B	146	LEU
2	B	151	VAL
2	B	162	VAL
2	B	166	MET
2	B	174	LYS
2	B	182	ILE
2	B	196	THR
2	B	215	SER
2	B	224	VAL
2	B	234	ILE
2	B	240	PHE
2	B	247	ASN
2	B	249	THR
2	B	253	CYS
2	B	254	ASN
2	B	260	MET
2	B	261	VAL
2	B	265	LEU
2	B	266	LEU
2	B	276	ILE
2	B	279	LEU
3	C	14	GLN
3	C	17	LEU
3	C	18	VAL
3	C	22	ASP
3	C	25	ARG
3	C	28	SER
3	C	30	ILE
3	C	31	LEU
3	C	34	ILE
3	C	37	ARG
3	C	42	CYS
3	C	43	PHE
3	C	49	ILE
3	C	64	PHE
3	C	65	ILE
3	C	71	GLN
3	C	72	GLU
3	C	83	ARG
3	C	84	ILE
3	C	88	VAL

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Mol	Chain	Res	Type
3	C	93	LEU
3	C	96	PHE
3	C	98	SER
3	C	101	MET
3	C	111	CYS
3	C	112	TYR
3	C	122	PHE
3	C	125	GLU
3	C	129	VAL
3	C	140	GLU
3	C	141	GLU
3	C	145	PHE
3	C	146	ASP
3	C	150	THR
3	C	151	ASN
3	C	158	LEU
3	C	163	LEU
3	C	164	ARG
3	C	167	PHE
3	C	169	GLU
3	C	170	LEU
3	C	172	MET
3	C	180	THR
3	C	181	MET
3	C	184	ASP
3	C	189	ARG
3	C	199	SER
3	C	203	TYR
3	C	208	ASP
3	C	209	LEU
3	C	215	CYS
3	C	221	ASN
3	C	222	ARG
3	C	227	LEU
3	C	228	LEU
3	C	236	VAL
3	C	237	LEU
3	C	240	LYS
3	C	242	SER
3	C	246	ASP
3	C	248	ARG
3	C	254	GLN

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Mol	Chain	Res	Type
3	C	255	TYR
3	C	259	ASN
3	C	260	GLU
3	C	264	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	42	ASN
1	A	102	ASN
1	A	122	HIS
1	A	143	HIS
1	A	182	HIS
1	A	205	GLN
1	A	206	GLN
1	A	235	ASN
1	A	259	HIS
2	B	14	ASN
2	B	21	ASN
2	B	60	GLN
2	B	62	ASN
2	B	65	ASN
2	B	76	ASN
2	B	254	ASN
3	C	14	GLN
3	C	26	ASN
3	C	60	GLN
3	C	62	ASN
3	C	71	GLN
3	C	214	HIS
3	C	221	ASN
3	C	247	ASN
3	C	259	ASN

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 carbohydrates 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	264/270 (97%)	0.18	11 (4%)	40	26	40, 69, 79, 79	0
2	B	278/286 (97%)	0.28	20 (7%)	18	10	39, 68, 79, 80	0
3	C	264/282 (93%)	0.25	9 (3%)	49	34	38, 71, 79, 79	0
All	All	806/838 (96%)	0.24	40 (4%)	32	19	38, 69, 79, 80	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	280	SER	4.3
2	B	124	SER	4.3
2	B	75	GLU	3.9
2	B	37	ASP	3.8
2	B	214	ALA	3.8
2	B	218	THR	3.6
2	B	123	SER	3.5
3	C	181	MET	3.4
2	B	47	LEU	3.4
1	A	134	ALA	3.3
2	B	125	SER	3.1
2	B	215	SER	3.0
2	B	49	ASN	2.9
2	B	143	TRP	2.9
2	B	223	ASN	2.8
1	A	70	LEU	2.8
1	A	128	ASP	2.8
1	A	189	THR	2.8
1	A	186	ALA	2.7
2	B	227	MET	2.7
2	B	220	GLU	2.7
1	A	92	LYS	2.6
3	C	127	GLY	2.6

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
3	C	272	CYS	2.6
3	C	173	THR	2.5
3	C	184	ASP	2.5
2	B	217	SER	2.5
2	B	226	HIS	2.5
2	B	46	LYS	2.5
1	A	132	LEU	2.4
3	C	178	GLN	2.3
3	C	259	ASN	2.3
3	C	113	GLN	2.2
1	A	129	CYS	2.2
3	C	116	GLY	2.2
2	B	145	ASP	2.1
1	A	105	SER	2.1
1	A	191	LYS	2.0
1	A	93	THR	2.0
2	B	74	ALA	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.