Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 02:46 am BST

PDB ID	:	1K5H
Title	:	1-deoxy-D-xylulose-5-phosphate reductoisomerase
Authors	:	Reuter, K.; Sanderbrand, S.; Jomaa, H.; Wiesner, J.; Steinbrecher, I.; Beck, E.; Hintz, M.; Klebe, G.; Stubbs, M.T.
Deposited on	:	2001-10-10
Resolution	:	2.50 Å(reported)

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

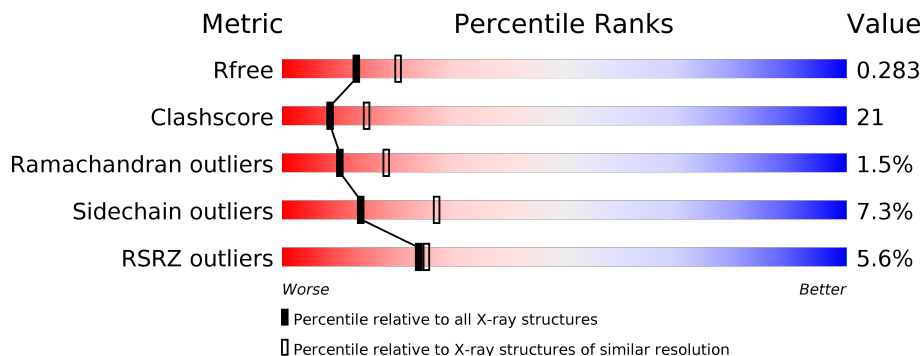|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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		0.283
Clashscore		21
Ramachandran outliers		1.5%
Sidechain outliers		7.3%
RSRZ outliers		5.6%

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	398	3% 64% 31% 5% ·
1	B	398	8% 59% 34% · · ·
1	C	398	6% 62% 35% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9126 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 1-deoxy-D-xylulose-5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total 3030	C 1892	N 534	O 577	S 27	0	0	0
1	B	391	Total 2978	C 1860	N 526	O 567	S 25	0	0	0
1	C	398	Total 3030	C 1892	N 534	O 577	S 27	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total 23	O 23	0	0
2	B	25	Total 25	O 25	0	0
2	C	40	Total 40	O 40	0	0

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.
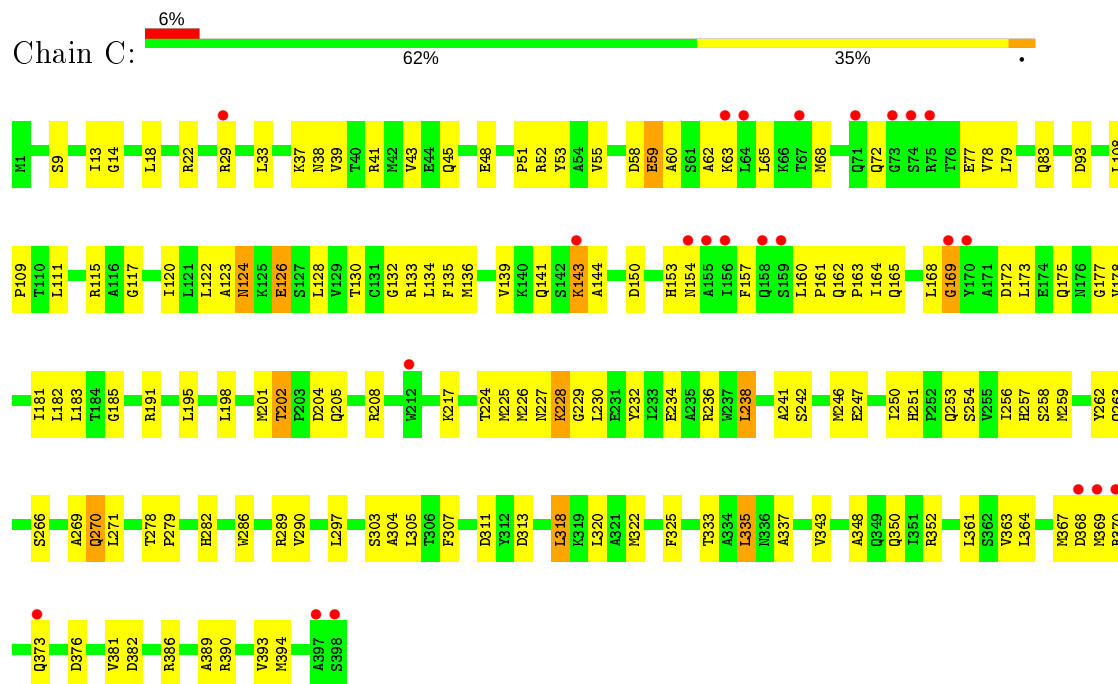
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate reductoisomerase
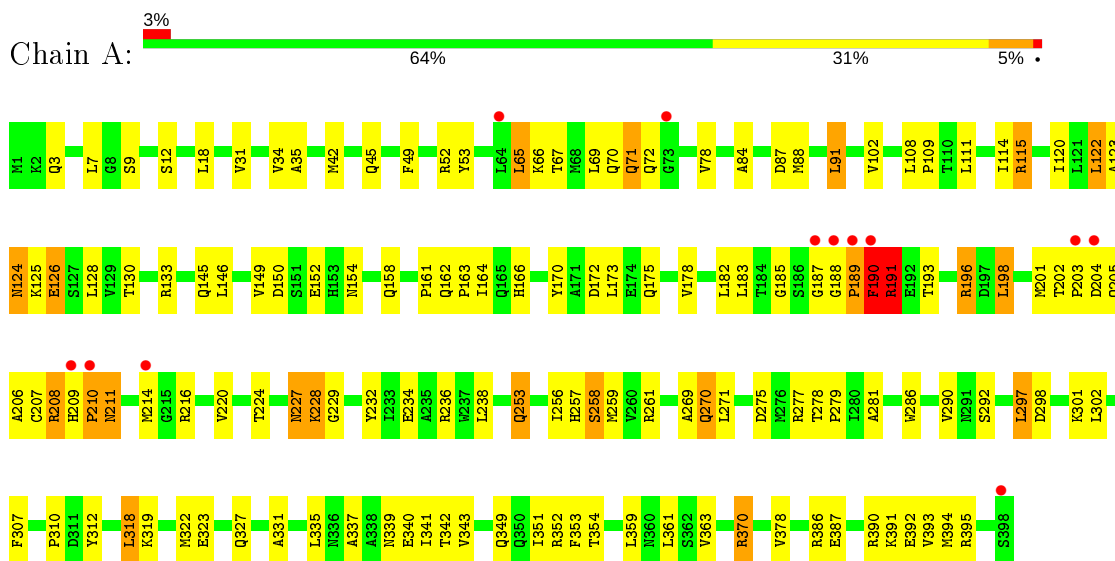
Chain A:

- Molecule 1: 1-deoxy-D-xylulose-5-phosphate reductoisomerase

Chain B:

● Molecule 1: 1-deoxy-D-xylulose-5-phosphate reductoisomerase

Chain C:
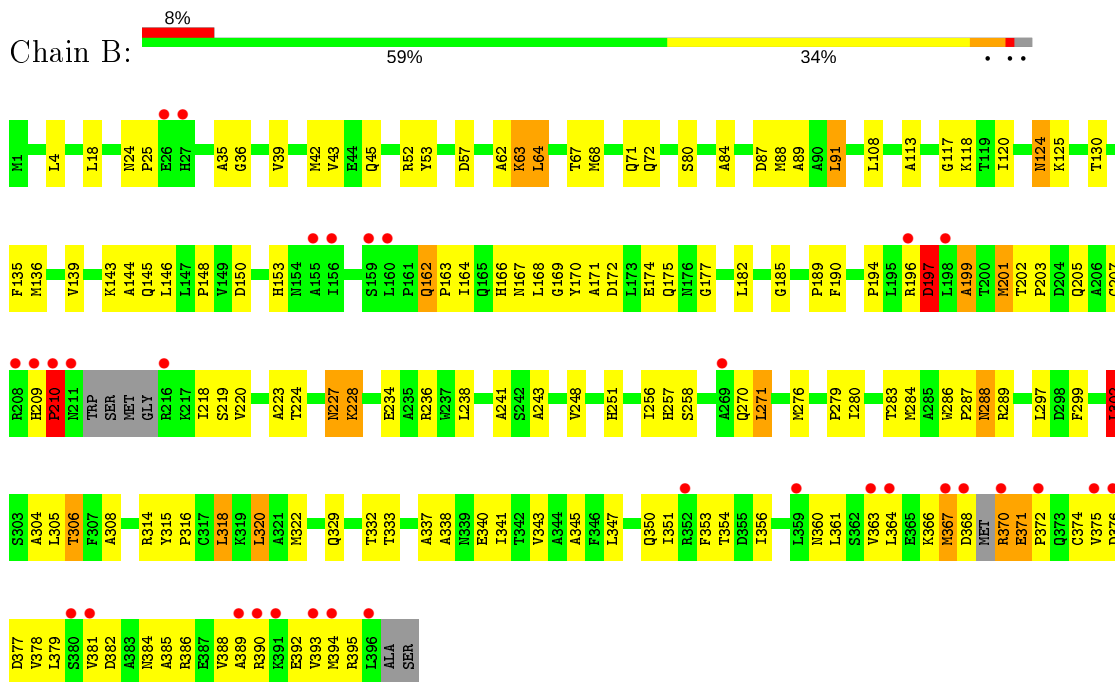
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.27Å 249.26Å 132.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.50 33.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.6 (33.45-2.50) 90.5 (33.45-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.10 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.284 0.233 , 0.283	Depositor DCC
R_{free} test set	5816 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9126	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, 0.333 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	0.35	0/3078	0.61	0/4171
1	B	0.36	0/3022	0.66	2/4094 (0.0%)
1	C	0.39	0/3078	0.64	0/4171
All	All	0.37	0/9178	0.64	2/12436 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	210	PRO	CA-N-CD	-14.82	90.75	111.50
1	B	302	LEU	CA-CB-CG	5.14	127.13	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	3030	0	3053	135	0
1	B	2978	0	3007	139	0
1	C	3030	0	3055	117	0
2	A	23	0	0	0	0
2	B	25	0	0	0	0
2	C	40	0	0	2	0
All	All	9126	0	9115	378	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 21.

All (378) 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:B:288:ASN:ND2	1:B:289:ARG:H	1.59	1.00
1:C:59:GLU:HA	1:C:62:ALA:HB3	1.46	0.97
1:B:210:PRO:HG3	1:B:219:SER:OG	1.64	0.97
1:A:208:ARG:H	1:A:208:ARG:HD2	1.30	0.96
1:A:256:ILE:HG12	1:A:271:LEU:HD22	1.52	0.91
1:C:202:THR:HG22	1:C:205:GLN:HG3	1.52	0.90
1:A:124:ASN:H	1:A:124:ASN:HD22	1.18	0.88
1:A:370:ARG:H	1:A:370:ARG:HD2	1.36	0.88
1:C:363:VAL:O	1:C:367:MET:HG2	1.72	0.87
1:B:288:ASN:HD22	1:B:289:ARG:N	1.72	0.86
1:B:288:ASN:HD22	1:B:289:ARG:H	0.87	0.85
1:A:297:LEU:HD21	1:A:302:LEU:HD21	1.60	0.82
1:C:181:ILE:HB	1:C:246:MET:HE2	1.60	0.82
1:A:256:ILE:HG12	1:A:271:LEU:CD2	2.08	0.82
1:C:256:ILE:HG12	1:C:271:LEU:HD22	1.61	0.82
1:B:130:THR:HG22	1:B:333:THR:HG23	1.62	0.81
1:B:220:VAL:HG11	1:B:343:VAL:HG13	1.61	0.80
1:A:211:ASN:ND2	1:A:214:MET:HB2	1.96	0.80
1:C:236:ARG:HD2	1:C:241:ALA:O	1.83	0.79
1:A:187:GLY:HA2	1:A:190:PHE:HA	1.65	0.78
1:B:227:ASN:ND2	1:B:228:LYS:H	1.82	0.78
1:A:257:HIS:HD2	1:A:270:GLN:HE22	1.31	0.78
1:B:118:LYS:O	1:B:120:ILE:HD12	1.85	0.76
1:A:278:THR:HB	1:A:279:PRO:HD3	1.68	0.76
1:C:177:GLY:HA2	1:C:263:GLN:NE2	2.01	0.76
1:A:319:LYS:HA	1:A:322:MET:HE2	1.68	0.75
1:B:218:ILE:H	1:B:218:ILE:HD12	1.51	0.75
1:B:146:LEU:HB2	1:B:168:LEU:HD12	1.69	0.73
1:B:39:VAL:O	1:B:43:VAL:HG23	1.89	0.73
1:B:52:ARG:HD2	1:B:53:TYR:CE1	2.23	0.73
1:C:52:ARG:HD2	1:C:53:TYR:HE1	1.52	0.73
1:C:52:ARG:HD2	1:C:53:TYR:CE1	2.24	0.73
1:A:204:ASP:OD1	1:A:205:GLN:HG3	1.88	0.72
1:A:257:HIS:CD2	1:A:270:GLN:HE22	2.07	0.72
1:C:41:ARG:HH11	1:C:41:ARG:HG2	1.53	0.72
1:A:120:ILE:HB	1:A:146:LEU:HD23	1.72	0.71
1:A:193:THR:HG23	1:A:196:ARG:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ILE:HB	1:C:246:MET:CE	2.20	0.71
1:A:208:ARG:CD	1:A:208:ARG:H	2.01	0.71
1:C:39:VAL:O	1:C:43:VAL:HG23	1.90	0.70
1:B:377:ASP:O	1:B:381:VAL:HG23	1.92	0.70
1:C:172:ASP:OD2	1:C:175:GLN:HG2	1.91	0.69
1:B:271:LEU:N	1:B:271:LEU:HD23	2.08	0.69
1:B:299:PHE:HA	1:B:302:LEU:HD22	1.74	0.69
1:B:338:ALA:HB1	1:B:363:VAL:HG21	1.74	0.69
1:C:256:ILE:HG12	1:C:271:LEU:CD2	2.23	0.69
1:C:133:ARG:HH11	1:C:133:ARG:HG3	1.58	0.68
1:B:148:PRO:HG3	1:B:238:LEU:HD21	1.74	0.68
1:A:203:PRO:HD3	1:C:373:GLN:O	1.94	0.68
1:A:12:SER:HB2	1:A:208:ARG:HG3	1.76	0.67
1:A:359:LEU:O	1:A:363:VAL:HG23	1.94	0.67
1:A:370:ARG:H	1:A:370:ARG:CD	2.07	0.67
1:A:319:LYS:O	1:A:323:GLU:HG3	1.95	0.67
1:B:360:ASN:O	1:B:364:LEU:HD23	1.95	0.67
1:A:253:GLN:H	1:A:253:GLN:CD	1.97	0.67
1:A:124:ASN:N	1:A:124:ASN:HD22	1.86	0.67
1:C:143:LYS:HA	1:C:143:LYS:NZ	2.10	0.67
1:B:305:LEU:HB2	1:C:305:LEU:HB2	1.75	0.66
1:A:188:GLY:H	1:A:189:PRO:C	1.98	0.66
1:A:84:ALA:O	1:A:88:MET:HG2	1.95	0.66
1:A:198:LEU:HD22	1:C:111:LEU:HD23	1.79	0.66
1:B:389:ALA:O	1:B:393:VAL:HG23	1.96	0.66
1:B:227:ASN:N	1:B:227:ASN:HD22	1.93	0.65
1:A:390:ARG:HA	1:A:393:VAL:HG12	1.78	0.65
1:A:162:GLN:HB3	1:A:163:PRO:HD3	1.78	0.65
1:A:3:GLN:HB3	1:A:31:VAL:CG2	2.26	0.65
1:C:143:LYS:HA	1:C:143:LYS:HZ3	1.62	0.65
1:A:318:LEU:HD22	1:A:322:MET:HE1	1.79	0.65
1:A:9:SER:HB2	1:A:45:GLN:HE22	1.62	0.65
1:A:196:ARG:HA	1:A:196:ARG:HE	1.61	0.65
1:B:185:GLY:HA3	1:B:228:LYS:HD3	1.79	0.64
1:B:288:ASN:ND2	1:B:289:ARG:N	2.40	0.64
1:B:36:GLY:HA2	1:B:57:ASP:HB2	1.80	0.64
1:A:208:ARG:HD2	1:A:208:ARG:N	2.11	0.63
1:B:62:ALA:HB2	1:B:80:SER:HB3	1.79	0.63
1:A:256:ILE:HA	1:A:271:LEU:HD22	1.81	0.63
1:A:185:GLY:HA3	1:A:228:LYS:HE2	1.81	0.62
1:C:185:GLY:HA3	1:C:228:LYS:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD12	1:B:45:GLN:NE2	2.13	0.62
1:C:22:ARG:HD3	1:C:48:GLU:OE1	1.99	0.62
1:C:202:THR:HG23	1:C:204:ASP:H	1.64	0.61
1:A:172:ASP:OD1	1:A:175:GLN:HG3	2.00	0.61
1:C:154:ASN:HD21	1:C:282:HIS:CD2	2.17	0.61
1:B:67:THR:O	1:B:71:GLN:HG2	1.99	0.61
1:A:210:PRO:HB3	1:C:115:ARG:HB3	1.82	0.61
1:C:55:VAL:HG22	1:C:79:LEU:HB2	1.82	0.61
1:A:124:ASN:H	1:A:124:ASN:ND2	1.92	0.61
1:C:29:ARG:HH11	1:C:29:ARG:HG2	1.66	0.60
1:C:253:GLN:O	1:C:254:SER:HB2	2.02	0.59
1:C:217:LYS:HG3	1:C:343:VAL:HG11	1.85	0.59
1:B:175:GLN:HA	1:B:175:GLN:HE21	1.68	0.59
1:C:165:GLN:NE2	1:C:286:TRP:HE1	2.00	0.59
1:C:227:ASN:OD1	1:C:228:LYS:N	2.35	0.58
1:B:251:HIS:HD2	1:B:306:THR:O	1.86	0.58
1:B:251:HIS:HE1	1:B:256:ILE:H	1.51	0.58
1:C:278:THR:HB	1:C:279:PRO:CD	2.34	0.58
1:A:327:GLN:HB2	1:A:331:ALA:CB	2.34	0.58
1:B:372:PRO:HB3	1:B:378:VAL:HG22	1.86	0.57
1:B:87:ASP:O	1:B:91:LEU:HD13	2.05	0.57
1:B:384:ASN:O	1:B:388:VAL:HG23	2.05	0.57
1:B:236:ARG:NH2	1:B:243:ALA:HB2	2.21	0.56
1:B:370:ARG:HG2	1:B:371:GLU:N	2.19	0.56
1:C:136:MET:CE	1:C:169:GLY:HA2	2.35	0.56
1:C:133:ARG:NH1	1:C:133:ARG:HG3	2.18	0.56
1:C:386:ARG:O	1:C:390:ARG:HG3	2.05	0.56
1:C:59:GLU:HA	1:C:62:ALA:CB	2.29	0.56
1:C:177:GLY:HA2	1:C:263:GLN:HE21	1.70	0.56
1:B:366:LYS:NZ	1:B:395:ARG:HH22	2.04	0.56
1:C:128:LEU:CD1	1:C:238:LEU:HD13	2.36	0.56
1:C:182:LEU:HD23	1:C:247:GLU:HB2	1.86	0.56
1:A:387:GLU:HG3	1:A:391:LYS:HE3	1.87	0.56
1:C:154:ASN:HD21	1:C:282:HIS:HD2	1.54	0.56
1:B:162:GLN:CD	1:C:162:GLN:HG3	2.26	0.56
1:B:388:VAL:O	1:B:392:GLU:HG2	2.06	0.55
1:B:125:LYS:HD2	1:B:234:GLU:OE1	2.05	0.55
1:B:314:ARG:C	1:B:316:PRO:HD3	2.27	0.55
1:C:128:LEU:HD11	1:C:238:LEU:HD13	1.89	0.55
1:C:257:HIS:HD2	1:C:270:GLN:HE22	1.55	0.55
1:C:173:LEU:HD22	1:C:178:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HD11	1:C:259:MET:HE1	1.87	0.55
1:A:202:THR:HB	1:A:203:PRO:HD2	1.88	0.55
1:A:67:THR:O	1:A:71:GLN:HG2	2.07	0.55
1:A:337:ALA:HB1	1:A:386:ARG:HG3	1.90	0.54
1:B:190:PHE:CZ	1:B:201:MET:HG2	2.42	0.54
1:B:218:ILE:CD1	1:B:218:ILE:H	2.19	0.54
1:A:259:MET:HG2	1:A:269:ALA:HB2	1.89	0.54
1:A:227:ASN:ND2	1:A:228:LYS:N	2.56	0.54
1:B:218:ILE:HD12	1:B:218:ILE:N	2.21	0.54
1:C:236:ARG:NH2	1:C:325:PHE:CD2	2.76	0.54
1:B:341:ILE:HB	1:B:389:ALA:HB1	1.89	0.54
1:A:256:ILE:CG1	1:A:271:LEU:HD22	2.33	0.54
1:A:370:ARG:N	1:A:370:ARG:HD2	2.14	0.54
1:C:13:ILE:HD13	1:C:123:ALA:HB1	1.90	0.53
1:B:139:VAL:O	1:B:143:LYS:N	2.40	0.53
1:C:135:PHE:O	1:C:139:VAL:HG23	2.09	0.53
1:C:134:LEU:HD21	1:C:373:GLN:O	2.09	0.53
1:B:124:ASN:H	1:B:124:ASN:HD22	1.55	0.53
1:C:369:MET:SD	1:C:381:VAL:HA	2.49	0.53
1:A:298:ASP:OD2	1:A:301:LYS:HD3	2.09	0.53
1:B:227:ASN:HD22	1:B:228:LYS:H	1.52	0.53
1:B:270:GLN:HE21	1:C:266:SER:HB2	1.74	0.53
1:A:18:LEU:HD22	1:A:49:PHE:CE1	2.44	0.53
1:C:389:ALA:O	1:C:393:VAL:HG23	2.09	0.53
1:A:87:ASP:O	1:A:91:LEU:HD13	2.09	0.52
1:B:124:ASN:N	1:B:124:ASN:HD22	2.07	0.52
1:B:148:PRO:CG	1:B:238:LEU:HD21	2.39	0.52
1:C:253:GLN:H	1:C:253:GLN:CD	2.12	0.52
1:B:386:ARG:O	1:B:390:ARG:NH1	2.42	0.52
1:C:117:GLY:HA2	1:C:144:ALA:HB2	1.89	0.52
1:B:320:LEU:HD11	1:B:361:LEU:HA	1.90	0.52
1:A:256:ILE:HG12	1:A:271:LEU:HD21	1.92	0.52
1:B:189:PRO:HD2	1:B:223:ALA:HA	1.92	0.52
1:C:37:LYS:O	1:C:39:VAL:HG23	2.09	0.52
1:A:122:LEU:HD22	1:A:124:ASN:ND2	2.24	0.52
1:C:162:GLN:HB2	1:C:163:PRO:HD3	1.92	0.52
1:B:84:ALA:O	1:B:88:MET:HG2	2.09	0.52
1:C:311:ASP:HB3	1:C:313:ASP:OD1	2.10	0.52
1:C:33:LEU:HD12	1:C:51:PRO:HG3	1.92	0.52
1:C:65:LEU:HD13	1:C:65:LEU:C	2.30	0.52
1:A:70:GLN:C	1:A:72:GLN:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLN:HA	1:B:175:GLN:NE2	2.25	0.52
1:B:236:ARG:HD2	1:B:241:ALA:O	2.11	0.51
1:B:64:LEU:O	1:B:68:MET:HG3	2.10	0.51
1:A:130:THR:HB	1:A:378:VAL:CG1	2.40	0.51
1:B:338:ALA:CB	1:B:363:VAL:HG21	2.39	0.51
1:A:253:GLN:N	1:A:253:GLN:CD	2.63	0.51
1:C:150:ASP:OD2	1:C:153:HIS:ND1	2.44	0.51
1:A:125:LYS:HD3	1:A:150:ASP:HB2	1.92	0.51
1:B:172:ASP:OD2	1:B:175:GLN:HB2	2.11	0.51
1:C:282:HIS:HE1	2:C:423:HOH:O	1.93	0.51
1:A:130:THR:HB	1:A:378:VAL:HG11	1.92	0.51
1:B:36:GLY:CA	1:B:57:ASP:HB2	2.40	0.51
1:C:172:ASP:HB3	1:C:175:GLN:CG	2.41	0.51
1:A:3:GLN:HB3	1:A:31:VAL:HG23	1.93	0.51
1:B:227:ASN:ND2	1:B:228:LYS:N	2.54	0.50
1:B:370:ARG:HD2	1:B:370:ARG:N	2.25	0.50
1:C:172:ASP:HB3	1:C:175:GLN:HG3	1.93	0.50
1:B:35:ALA:HB2	1:B:42:MET:HE2	1.93	0.50
1:A:154:ASN:O	1:A:158:GLN:HG3	2.12	0.50
1:B:361:LEU:HD22	1:B:361:LEU:O	2.12	0.50
1:B:374:CYS:C	1:B:376:ASP:H	2.14	0.50
1:B:366:LYS:HZ1	1:B:395:ARG:HH22	1.57	0.50
1:B:210:PRO:HA	1:B:219:SER:HB3	1.93	0.50
1:B:196:ARG:NH2	1:B:199:ALA:HB3	2.26	0.50
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.75	0.50
1:A:387:GLU:CG	1:A:391:LYS:HE3	2.41	0.50
1:B:374:CYS:HB3	1:B:377:ASP:OD2	2.11	0.50
1:B:297:LEU:HD12	1:B:299:PHE:CE1	2.47	0.50
1:C:259:MET:HG2	1:C:269:ALA:HB2	1.94	0.50
1:B:304:ALA:HB1	1:C:304:ALA:HB1	1.94	0.50
1:C:124:ASN:N	1:C:124:ASN:HD22	2.10	0.49
1:A:188:GLY:H	1:A:190:PHE:N	2.10	0.49
1:A:319:LYS:HA	1:A:322:MET:CE	2.40	0.49
1:B:166:HIS:CD2	1:B:286:TRP:HZ2	2.29	0.49
1:B:135:PHE:O	1:B:139:VAL:HG23	2.13	0.49
1:B:276:MET:HE2	1:B:276:MET:HA	1.93	0.49
1:B:318:LEU:O	1:B:322:MET:HG3	2.12	0.49
1:B:341:ILE:HG13	1:B:389:ALA:HB3	1.93	0.49
1:C:124:ASN:H	1:C:124:ASN:HD22	1.60	0.49
1:C:58:ASP:OD2	1:C:60:ALA:HB3	2.13	0.49
1:A:150:ASP:OD2	1:A:152:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:HD22	1:A:214:MET:HB2	1.71	0.49
1:A:102:VAL:HA	1:A:126:GLU:OE1	2.12	0.49
1:A:18:LEU:HD11	1:A:45:GLN:NE2	2.27	0.49
1:A:392:GLU:O	1:A:395:ARG:HG2	2.13	0.49
1:B:89:ALA:HB1	1:B:113:ALA:HB2	1.95	0.49
1:C:160:LEU:HD13	1:C:164:ILE:HG21	1.95	0.49
1:A:18:LEU:HD22	1:A:49:PHE:CD1	2.48	0.48
1:B:251:HIS:CD2	1:B:306:THR:O	2.66	0.48
1:C:259:MET:HG2	1:C:269:ALA:CB	2.43	0.48
1:A:161:PRO:CG	1:A:164:ILE:HD12	2.43	0.48
1:A:229:GLY:O	1:A:232:TYR:HB3	2.14	0.48
1:A:281:ALA:HB2	1:A:292:SER:HB3	1.95	0.48
1:B:337:ALA:O	1:B:340:GLU:HB2	2.13	0.48
1:A:188:GLY:N	1:A:190:PHE:N	2.62	0.48
1:A:209:HIS:ND1	1:A:210:PRO:HD2	2.28	0.48
1:C:130:THR:HG22	1:C:333:THR:HA	1.95	0.48
1:A:125:LYS:HB2	1:A:234:GLU:OE1	2.13	0.48
1:B:167:ASN:HA	1:B:170:TYR:CZ	2.49	0.48
1:B:341:ILE:HG22	1:B:393:VAL:HG21	1.96	0.48
1:B:150:ASP:OD1	1:B:153:HIS:ND1	2.46	0.48
1:C:124:ASN:ND2	1:C:124:ASN:H	2.11	0.48
1:B:62:ALA:CB	1:B:80:SER:HB3	2.43	0.48
1:C:136:MET:HE3	1:C:169:GLY:HA2	1.96	0.47
1:C:153:HIS:HE1	1:C:234:GLU:OE1	1.96	0.47
1:B:374:CYS:C	1:B:376:ASP:N	2.67	0.47
1:A:191:ARG:HD3	1:A:191:ARG:C	2.35	0.47
1:A:52:ARG:HD2	1:A:53:TYR:CE1	2.49	0.47
1:B:337:ALA:HB2	1:B:382:ASP:OD1	2.13	0.47
1:C:318:LEU:HD22	1:C:322:MET:HE3	1.96	0.47
1:A:220:VAL:HG11	1:A:343:VAL:HG13	1.97	0.47
1:A:216:ARG:O	1:A:220:VAL:HG23	2.15	0.47
1:B:361:LEU:HD13	1:B:361:LEU:C	2.35	0.47
1:C:202:THR:HG23	1:C:204:ASP:N	2.30	0.47
1:A:189:PRO:O	1:A:191:ARG:N	2.47	0.47
1:A:318:LEU:HD22	1:A:322:MET:CE	2.45	0.47
1:B:194:PRO:HG2	1:B:197:ASP:HB2	1.97	0.47
1:C:157:PHE:CD1	1:C:168:LEU:HD11	2.50	0.46
1:A:122:LEU:HD22	1:A:124:ASN:HD21	1.81	0.46
1:A:340:GLU:HG3	1:A:386:ARG:NH2	2.30	0.46
1:C:122:LEU:HD12	1:C:124:ASN:HD21	1.81	0.46
1:C:18:LEU:HD12	1:C:45:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ARG:NH1	1:C:41:ARG:HG2	2.24	0.46
1:A:216:ARG:NH1	1:C:83:GLN:HE21	2.14	0.46
1:A:162:GLN:HG3	1:A:166:HIS:HD2	1.80	0.46
1:A:173:LEU:HB3	1:A:178:VAL:HB	1.98	0.46
1:A:145:GLN:NE2	1:A:286:TRP:CH2	2.84	0.46
1:C:191:ARG:HD3	2:C:430:HOH:O	2.16	0.46
1:A:108:LEU:HB2	1:A:109:PRO:HD3	1.98	0.46
1:A:352:ARG:HB2	1:A:352:ARG:HH11	1.80	0.46
1:A:35:ALA:HB3	1:A:42:MET:HE2	1.97	0.46
1:B:271:LEU:HD11	1:C:259:MET:CE	2.46	0.46
1:B:227:ASN:N	1:B:227:ASN:ND2	2.61	0.46
1:A:206:ALA:HA	1:A:208:ARG:CD	2.46	0.46
1:C:318:LEU:HD13	1:C:322:MET:HE3	1.97	0.46
1:C:335:LEU:HG	1:C:364:LEU:HD11	1.97	0.46
1:B:256:ILE:HA	1:B:271:LEU:HB3	1.99	0.45
1:C:318:LEU:HD22	1:C:322:MET:CE	2.46	0.45
1:A:190:PHE:N	1:A:190:PHE:CD1	2.84	0.45
1:A:259:MET:HG2	1:A:269:ALA:CB	2.46	0.45
1:C:224:THR:O	1:C:225:MET:HB2	2.16	0.45
1:C:29:ARG:HH11	1:C:29:ARG:CG	2.29	0.45
1:A:227:ASN:ND2	1:A:228:LYS:H	2.13	0.45
1:B:117:GLY:HA2	1:B:144:ALA:HB2	1.98	0.45
1:B:145:GLN:HE22	1:B:166:HIS:HA	1.81	0.45
1:A:170:TYR:CD1	1:A:170:TYR:N	2.84	0.45
1:A:390:ARG:O	1:A:393:VAL:HG12	2.17	0.45
1:A:164:ILE:HD13	1:A:173:LEU:HD23	1.99	0.45
1:A:128:LEU:CD1	1:A:238:LEU:HG	2.46	0.45
1:A:270:GLN:C	1:A:271:LEU:HD23	2.36	0.45
1:A:327:GLN:HB2	1:A:331:ALA:HB2	1.98	0.45
1:B:136:MET:CE	1:B:169:GLY:HA3	2.46	0.45
1:B:177:GLY:HA3	1:C:289:ARG:HB2	1.99	0.45
1:B:251:HIS:CE1	1:B:256:ILE:H	2.32	0.45
1:A:275:ASP:OD1	1:A:277:ARG:HD3	2.16	0.45
1:B:257:HIS:HD2	1:B:270:GLN:OE1	1.99	0.45
1:C:120:ILE:N	1:C:120:ILE:HD12	2.32	0.45
1:C:168:LEU:O	1:C:169:GLY:C	2.55	0.45
1:B:207:CYS:C	1:B:209:HIS:H	2.21	0.45
1:C:226:MET:O	1:C:230:LEU:HG	2.17	0.45
1:C:29:ARG:HB2	1:C:29:ARG:CZ	2.47	0.45
1:C:77:GLU:HG3	1:C:78:VAL:H	1.82	0.45
1:C:198:LEU:HA	1:C:201:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:VAL:HG11	1:B:318:LEU:HD11	1.99	0.44
1:B:271:LEU:N	1:B:271:LEU:CD2	2.79	0.44
1:A:352:ARG:NH1	1:A:352:ARG:CB	2.81	0.44
1:B:210:PRO:HD3	1:B:219:SER:CB	2.47	0.44
1:A:310:PRO:HG2	1:A:312:TYR:CZ	2.53	0.44
1:A:161:PRO:HG2	1:A:164:ILE:HD12	1.99	0.44
1:B:175:GLN:CA	1:B:175:GLN:HE21	2.29	0.44
1:A:65:LEU:HD13	1:A:78:VAL:HG21	1.99	0.44
1:A:66:LYS:O	1:A:70:GLN:HB2	2.18	0.44
1:B:224:THR:HG22	1:B:353:PHE:CZ	2.53	0.43
1:B:367:MET:HE1	1:B:385:ALA:N	2.33	0.43
1:A:228:LYS:HZ2	1:A:228:LYS:HA	1.83	0.43
1:C:68:MET:O	1:C:72:GLN:HG2	2.17	0.43
1:B:279:PRO:O	1:B:283:THR:HG23	2.19	0.43
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.87	0.43
1:A:257:HIS:HD2	1:A:270:GLN:NE2	2.06	0.43
1:A:352:ARG:NH1	1:A:352:ARG:HB2	2.34	0.43
1:C:108:LEU:HB2	1:C:109:PRO:HD3	2.01	0.43
1:C:9:SER:HA	1:C:14:GLY:HA3	2.00	0.43
1:C:132:GLY:O	1:C:136:MET:HG2	2.19	0.43
1:C:182:LEU:HD12	1:C:259:MET:HB2	2.00	0.43
1:C:352:ARG:HH11	1:C:352:ARG:HG2	1.83	0.43
1:A:352:ARG:NE	1:A:354:THR:HG22	2.34	0.43
1:A:65:LEU:HD22	1:A:69:LEU:HG	2.01	0.43
1:B:356:ILE:HG22	1:B:360:ASN:ND2	2.34	0.43
1:C:229:GLY:O	1:C:232:TYR:HB3	2.17	0.43
1:A:162:GLN:CB	1:A:163:PRO:HD3	2.46	0.43
1:A:391:LYS:HA	1:A:394:MET:HE3	2.01	0.43
1:A:352:ARG:CZ	1:A:352:ARG:HB3	2.49	0.43
1:B:270:GLN:HE21	1:C:266:SER:CB	2.32	0.43
1:A:65:LEU:HD13	1:A:78:VAL:CG2	2.49	0.43
1:A:257:HIS:O	1:A:258:SER:CB	2.67	0.42
1:B:363:VAL:O	1:B:367:MET:HG2	2.19	0.42
1:C:257:HIS:CD2	1:C:270:GLN:HE22	2.33	0.42
1:A:297:LEU:HD23	1:A:298:ASP:N	2.33	0.42
1:A:256:ILE:HD12	1:A:307:PHE:HZ	1.84	0.42
1:A:342:THR:O	1:A:351:ILE:HD11	2.19	0.42
1:A:228:LYS:NZ	1:A:228:LYS:HA	2.34	0.42
1:B:315:TYR:N	1:B:316:PRO:HD3	2.33	0.42
1:B:345:ALA:O	1:B:350:GLN:HB2	2.19	0.42
1:A:310:PRO:HG2	1:A:312:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MET:HB2	1:B:284:MET:HE3	1.96	0.42
1:B:375:VAL:O	1:B:379:LEU:HG	2.19	0.42
1:C:59:GLU:O	1:C:63:LYS:N	2.34	0.42
1:B:167:ASN:HB2	1:B:171:ALA:HB2	2.01	0.42
1:B:35:ALA:HB2	1:B:42:MET:CE	2.49	0.42
1:C:236:ARG:HH11	1:C:242:SER:HA	1.84	0.42
1:A:114:ILE:O	1:A:115:ARG:C	2.58	0.42
1:B:196:ARG:HH22	1:B:199:ALA:HB3	1.84	0.42
1:B:182:LEU:N	1:B:182:LEU:HD12	2.35	0.42
1:B:356:ILE:O	1:B:360:ASN:ND2	2.52	0.42
1:B:394:MET:HA	1:B:394:MET:CE	2.50	0.42
1:B:24:ASN:N	1:B:25:PRO:CD	2.83	0.42
1:B:280:ILE:CG2	1:B:284:MET:HE3	2.50	0.42
1:A:188:GLY:N	1:A:189:PRO:C	2.70	0.42
1:B:108:LEU:HA	1:B:108:LEU:HD23	1.82	0.42
1:B:63:LYS:HE3	1:B:67:THR:OG1	2.19	0.42
1:A:182:LEU:HD11	1:A:261:ARG:HB2	2.03	0.41
1:A:339:ASN:O	1:A:343:VAL:HG23	2.20	0.41
1:B:162:GLN:N	1:B:163:PRO:HD2	2.35	0.41
1:B:201:MET:HG3	1:B:205:GLN:OE1	2.20	0.41
1:C:161:PRO:HD3	1:C:262:TYR:OH	2.19	0.41
1:C:337:ALA:HB2	1:C:382:ASP:OD1	2.20	0.41
1:A:391:LYS:HA	1:A:394:MET:CE	2.50	0.41
1:B:203:PRO:HB3	1:B:347:LEU:HD23	2.02	0.41
1:B:36:GLY:C	1:B:57:ASP:HB2	2.41	0.41
1:C:250:ILE:O	1:C:307:PHE:HA	2.20	0.41
1:B:209:HIS:N	1:B:210:PRO:HD2	2.35	0.41
1:B:286:TRP:CD1	1:B:287:PRO:HA	2.55	0.41
1:C:202:THR:HG22	1:C:205:GLN:H	1.84	0.41
1:C:251:HIS:HE1	1:C:305:LEU:HD22	1.85	0.41
1:B:164:ILE:HD13	1:B:171:ALA:HB3	2.02	0.41
1:A:202:THR:HG22	1:C:373:GLN:HB3	2.02	0.41
1:A:341:ILE:HD13	1:A:386:ARG:HG2	2.03	0.41
1:C:236:ARG:NH1	1:C:242:SER:HA	2.36	0.41
1:C:236:ARG:NH2	1:C:325:PHE:HD2	2.18	0.41
1:A:224:THR:HG22	1:A:353:PHE:CZ	2.55	0.41
1:A:7:LEU:HA	1:A:34:VAL:HB	2.03	0.41
1:A:123:ALA:HA	1:A:149:VAL:HB	2.03	0.41
1:B:207:CYS:C	1:B:210:PRO:HD2	2.41	0.41
1:B:124:ASN:N	1:B:124:ASN:ND2	2.69	0.41
1:B:136:MET:HE1	1:B:169:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PHE:H	1:A:190:PHE:HD1	1.61	0.41
1:A:18:LEU:CD1	1:A:45:GLN:NE2	2.84	0.41
1:B:199:ALA:HA	1:B:354:THR:HB	2.02	0.41
1:B:345:ALA:HB3	1:B:351:ILE:HD11	2.01	0.41
1:B:202:THR:OG1	1:B:205:GLN:HG3	2.21	0.40
1:B:210:PRO:HD3	1:B:219:SER:HB3	2.02	0.40
1:C:201:MET:HE3	1:C:205:GLN:HB3	2.02	0.40
1:A:281:ALA:CB	1:A:292:SER:HB3	2.52	0.40
1:B:314:ARG:HD3	1:B:315:TYR:CZ	2.56	0.40
1:C:122:LEU:CD1	1:C:124:ASN:HD21	2.34	0.40
1:C:348:ALA:HB3	1:C:350:GLN:HG2	2.01	0.40
1:B:329:GLN:HA	1:B:332:THR:OG1	2.22	0.40
1:B:385:ALA:O	1:B:386:ARG:C	2.59	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	396/398 (100%)	367 (93%)	21 (5%)	8 (2%)	7	12
1	B	385/398 (97%)	351 (91%)	29 (8%)	5 (1%)	12	21
1	C	396/398 (100%)	378 (96%)	13 (3%)	5 (1%)	12	21
All	All	1177/1194 (99%)	1096 (93%)	63 (5%)	18 (2%)	10	18

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	PHE
1	A	210	PRO
1	A	258	SER
1	A	349	GLN

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Mol	Chain	Res	Type
1	B	371	GLU
1	A	191	ARG
1	C	38	ASN
1	C	169	GLY
1	C	258	SER
1	A	211	ASN
1	B	197	ASP
1	A	71	GLN
1	B	199	ALA
1	C	126	GLU
1	B	308	ALA
1	B	367	MET
1	C	368	ASP
1	A	189	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	328/328 (100%)	302 (92%)	26 (8%)	12	24
1	B	323/328 (98%)	301 (93%)	22 (7%)	16	30
1	C	328/328 (100%)	305 (93%)	23 (7%)	15	29
All	All	979/984 (100%)	908 (93%)	71 (7%)	14	27

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

Mol	Chain	Res	Type
1	A	65	LEU
1	A	91	LEU
1	A	111	LEU
1	A	115	ARG
1	A	122	LEU
1	A	124	ASN
1	A	126	GLU
1	A	183	LEU

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Mol	Chain	Res	Type
1	A	190	PHE
1	A	191	ARG
1	A	196	ARG
1	A	198	LEU
1	A	201	MET
1	A	207	CYS
1	A	208	ARG
1	A	227	ASN
1	A	228	LYS
1	A	236	ARG
1	A	253	GLN
1	A	270	GLN
1	A	290	VAL
1	A	297	LEU
1	A	318	LEU
1	A	335	LEU
1	A	361	LEU
1	A	370	ARG
1	B	4	LEU
1	B	63	LYS
1	B	64	LEU
1	B	72	GLN
1	B	91	LEU
1	B	124	ASN
1	B	162	GLN
1	B	174	GLU
1	B	197	ASP
1	B	201	MET
1	B	210	PRO
1	B	227	ASN
1	B	228	LYS
1	B	258	SER
1	B	271	LEU
1	B	288	ASN
1	B	302	LEU
1	B	306	THR
1	B	318	LEU
1	B	320	LEU
1	B	368	ASP
1	B	370	ARG
1	C	59	GLU
1	C	93	ASP

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Mol	Chain	Res	Type
1	C	124	ASN
1	C	126	GLU
1	C	141	GLN
1	C	143	LYS
1	C	183	LEU
1	C	195	LEU
1	C	202	THR
1	C	208	ARG
1	C	228	LYS
1	C	238	LEU
1	C	270	GLN
1	C	290	VAL
1	C	297	LEU
1	C	303	SER
1	C	318	LEU
1	C	320	LEU
1	C	335	LEU
1	C	361	LEU
1	C	370	ARG
1	C	376	ASP
1	C	394	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	72	GLN
1	A	124	ASN
1	A	145	GLN
1	A	205	GLN
1	A	211	ASN
1	A	227	ASN
1	A	257	HIS
1	A	270	GLN
1	A	329	GLN
1	A	373	GLN
1	B	70	GLN
1	B	71	GLN
1	B	72	GLN
1	B	124	ASN
1	B	145	GLN
1	B	162	GLN

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Mol	Chain	Res	Type
1	B	165	GLN
1	B	175	GLN
1	B	227	ASN
1	B	251	HIS
1	B	257	HIS
1	B	270	GLN
1	B	288	ASN
1	B	291	ASN
1	B	384	ASN
1	C	3	GLN
1	C	71	GLN
1	C	83	GLN
1	C	124	ASN
1	C	145	GLN
1	C	165	GLN
1	C	257	HIS
1	C	282	HIS

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	398/398 (100%)	0.20	12 (3%)	50 53	40, 60, 99, 116	0
1	B	391/398 (98%)	0.36	32 (8%)	11 11	35, 64, 121, 144	0
1	C	398/398 (100%)	0.14	23 (5%)	23 24	25, 52, 91, 109	0
All	All	1187/1194 (99%)	0.23	67 (5%)	24 25	25, 58, 107, 144	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	MET	6.2
1	B	363	VAL	6.2
1	A	190	PHE	6.2
1	C	170	TYR	5.4
1	B	396	LEU	5.3
1	B	370	ARG	5.1
1	B	209	HIS	4.9
1	C	398	SER	4.8
1	A	203	PRO	4.6
1	B	372	PRO	4.5
1	B	394	MET	4.3
1	C	369	MET	4.2
1	B	381	VAL	4.0
1	C	63	LYS	3.8
1	B	210	PRO	3.8
1	B	364	LEU	3.4
1	C	64	LEU	3.4
1	B	211	ASN	3.3
1	C	212	TRP	3.3
1	B	393	VAL	3.0
1	C	75	ARG	2.9
1	A	398	SER	2.9
1	A	214	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	196	ARG	2.8
1	C	370	ARG	2.8
1	C	71	GLN	2.7
1	A	204	ASP	2.7
1	B	368	ASP	2.7
1	C	169	GLY	2.7
1	C	155	ALA	2.6
1	B	389	ALA	2.6
1	C	156	ILE	2.6
1	B	390	ARG	2.5
1	C	154	ASN	2.5
1	A	189	PRO	2.5
1	C	74	SER	2.5
1	C	368	ASP	2.5
1	B	160	LEU	2.4
1	C	73	GLY	2.4
1	B	208	ARG	2.4
1	A	188	GLY	2.4
1	B	391	LYS	2.4
1	B	269	ALA	2.4
1	A	187	GLY	2.4
1	B	380	SER	2.4
1	B	198	LEU	2.4
1	B	359	LEU	2.4
1	C	143	LYS	2.3
1	C	159	SER	2.3
1	B	26	GLU	2.3
1	C	397	ALA	2.3
1	A	209	HIS	2.3
1	B	27	HIS	2.3
1	B	375	VAL	2.2
1	B	352	ARG	2.2
1	A	210	PRO	2.2
1	A	64	LEU	2.2
1	B	156	ILE	2.2
1	C	67	THR	2.2
1	C	373	GLN	2.1
1	A	73	GLY	2.1
1	C	158	GLN	2.1
1	B	159	SER	2.1
1	B	155	ALA	2.0
1	B	216	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	29	ARG	2.0
1	B	376	ASP	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.