Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 09:03 AM EDT

PDB ID	:	2EEZ
Title	:	Crystal structure of alanine dehydrogenase from themus thermophilus
Authors	:	Kumarevel, T.S.; Karthe, P.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-02-19
Resolution	:	2.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

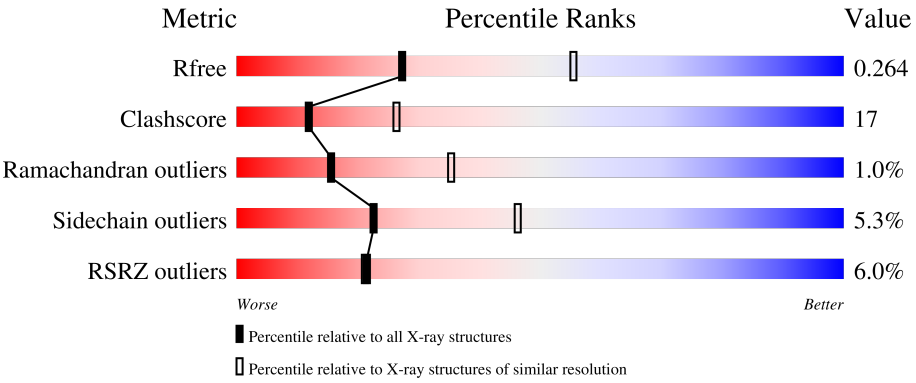
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	369	8% 62% 28% • 7%
1	C	369	5% 63% 27% • 7%
1	D	369	4% 63% 28% • 7%
1	E	369	6% 58% 33% • 7%
1	F	369	7% 64% 25% • 7%

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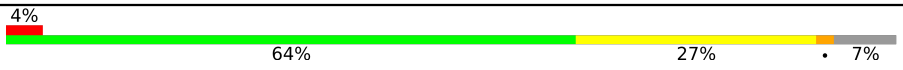
Mol	Chain	Length	Quality of chain
1	G	369	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15522 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 Alanine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2523	1604	438	472	9			
1	C	343	Total	C	N	O	S	0	0	0
			2523	1604	438	472	9			
1	D	343	Total	C	N	O	S	0	0	0
			2523	1604	438	472	9			
1	E	343	Total	C	N	O	S	0	0	0
			2523	1604	438	472	9			
1	F	343	Total	C	N	O	S	0	0	0
			2523	1604	438	472	9			
1	G	343	Total	C	N	O	S	0	0	0
			2523	1604	438	472	9			

- Molecule 2 is water.

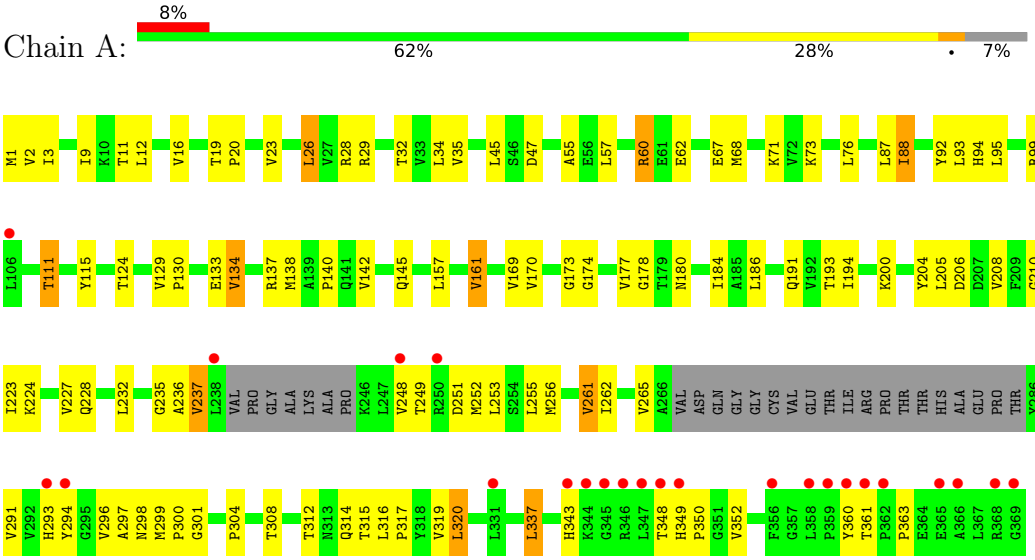
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	C	65	Total	O	0	0
			65	65		
2	D	65	Total	O	0	0
			65	65		
2	E	59	Total	O	0	0
			59	59		
2	F	64	Total	O	0	0
			64	64		
2	G	66	Total	O	0	0
			66	66		

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.

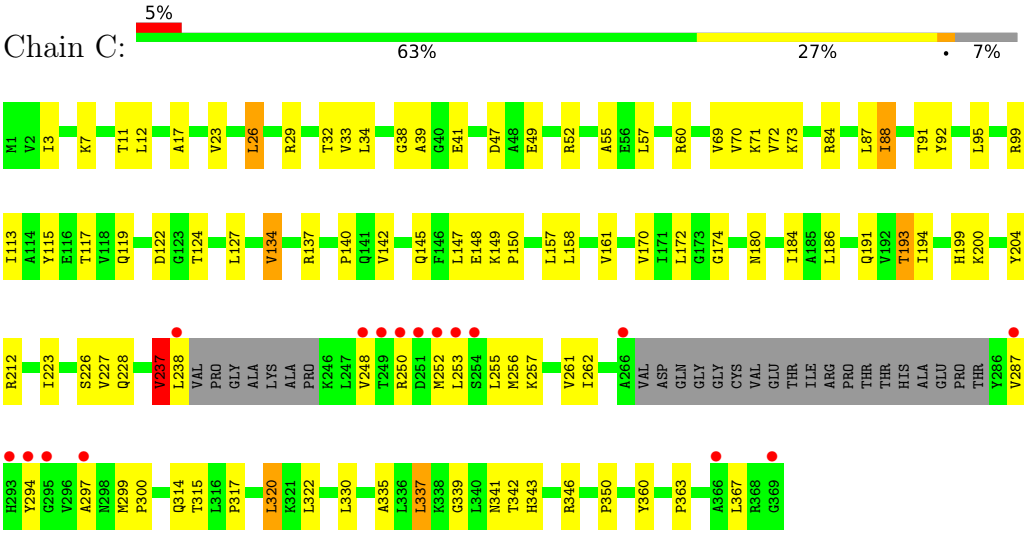
• Molecule 1: Alanine dehydrogenase

Chain A:



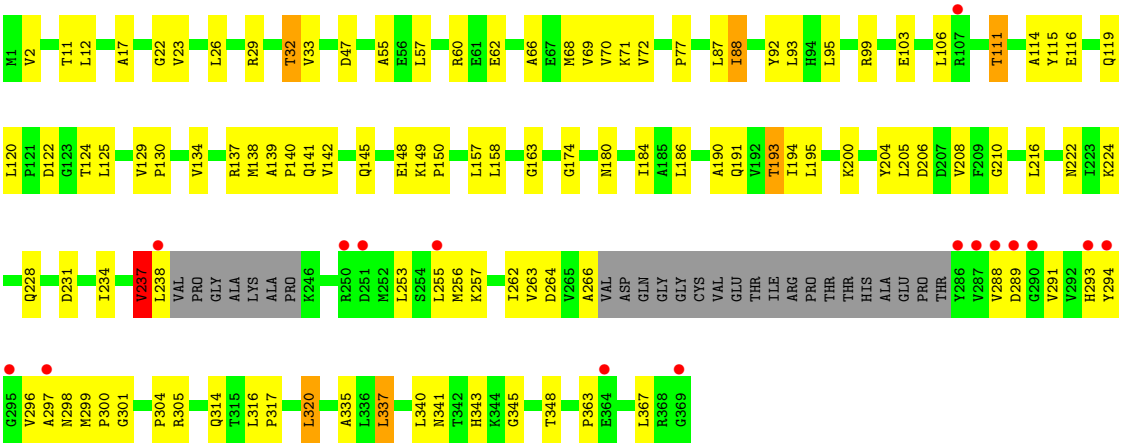
• Molecule 1: Alanine dehydrogenase

Chain C:

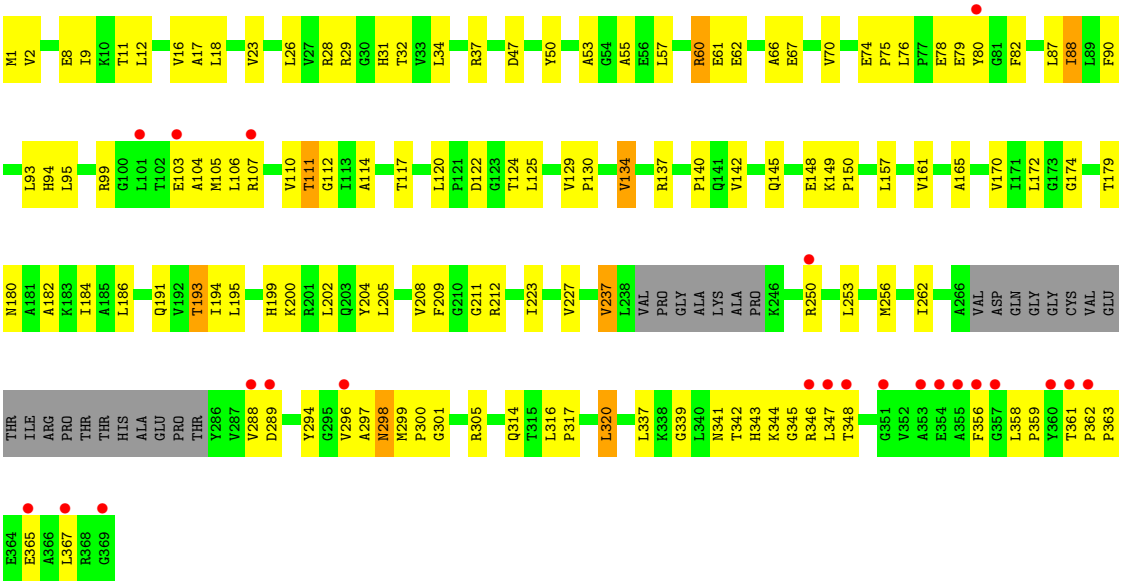


• Molecule 1: Alanine dehydrogenase

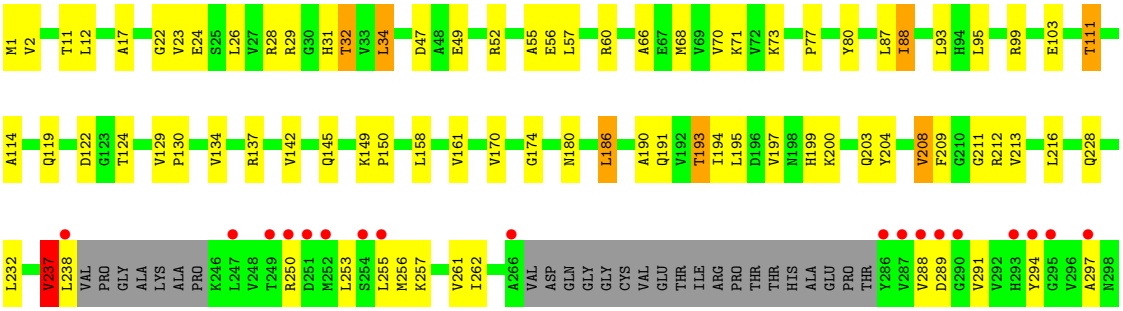
Chain D:

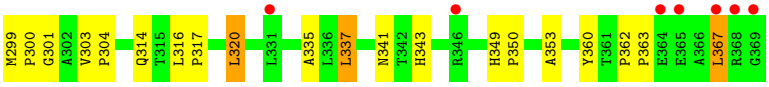


• Molecule 1: Alanine dehydrogenase

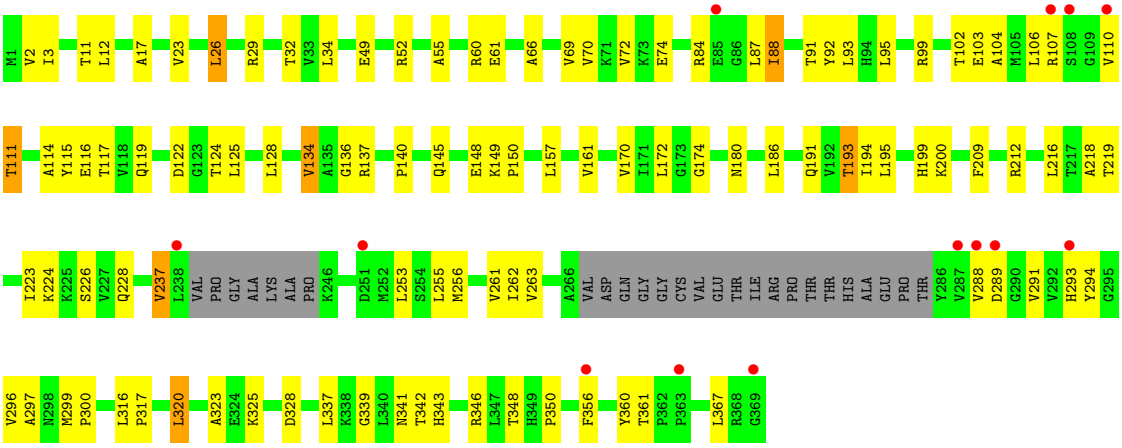


• Molecule 1: Alanine dehydrogenase





• Molecule 1: Alanine dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.94Å 133.24Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.71 39.75 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.95-2.71) 99.0 (39.75-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.66 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.264 0.219 , 0.264	Depositor DCC
R_{free} test set	3612 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15522	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	0/2562	0.62	0/3476
1	C	0.36	0/2562	0.63	0/3476
1	D	0.37	0/2562	0.65	0/3476
1	E	0.37	0/2562	0.62	0/3476
1	F	0.37	0/2562	0.63	0/3476
1	G	0.35	0/2562	0.63	0/3476
All	All	0.37	0/15372	0.63	0/20856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2523	0	2600	109	0
1	C	2523	0	2600	86	0
1	D	2523	0	2600	94	0
1	E	2523	0	2600	111	0
1	F	2523	0	2600	87	0
1	G	2523	0	2600	88	0
2	A	65	0	0	4	0
2	C	65	0	0	3	0
2	D	65	0	0	5	0
2	E	59	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	64	0	0	4	0
2	G	66	0	0	2	0
All	All	15522	0	15600	531	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 17.

All (531) 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:A:137:ARG:HE	1:A:180:ASN:HD22	1.07	1.01
1:A:256:MET:HE3	1:A:291:VAL:HG11	1.49	0.93
1:E:137:ARG:HE	1:E:180:ASN:HD22	1.09	0.93
1:G:256:MET:HE3	1:G:291:VAL:HG11	1.50	0.91
1:D:137:ARG:HE	1:D:180:ASN:HD22	1.14	0.91
1:G:137:ARG:HE	1:G:180:ASN:HD22	0.92	0.89
1:F:137:ARG:HE	1:F:180:ASN:HD22	1.10	0.89
1:A:191:GLN:NE2	1:C:191:GLN:NE2	2.22	0.88
1:D:256:MET:HE1	1:D:262:ILE:HD11	1.53	0.88
1:G:17:ALA:HB1	1:G:70:VAL:HG12	1.57	0.87
1:G:174:GLY:HA2	1:G:194:ILE:HD11	1.57	0.87
1:F:256:MET:HE3	1:F:291:VAL:HG11	1.57	0.87
1:E:145:GLN:NE2	2:E:376:HOH:O	2.09	0.86
1:A:137:ARG:NE	1:A:180:ASN:HD22	1.75	0.85
1:G:137:ARG:NE	1:G:180:ASN:HD22	1.75	0.84
1:C:95:LEU:HD12	1:C:341:ASN:HD22	1.43	0.84
1:A:200:LYS:NZ	1:E:124:THR:HG21	1.93	0.83
1:E:111:THR:HB	1:E:343:HIS:HD2	1.43	0.83
1:A:191:GLN:HE21	1:C:191:GLN:HE21	1.25	0.82
1:C:137:ARG:HE	1:C:180:ASN:HD22	1.28	0.81
1:A:191:GLN:NE2	1:C:191:GLN:HE21	1.78	0.81
1:G:111:THR:HB	1:G:343:HIS:HD2	1.44	0.81
1:C:124:THR:HG21	1:F:200:LYS:HZ1	1.45	0.81
1:C:124:THR:HG21	1:F:200:LYS:NZ	1.96	0.81
1:E:256:MET:HE3	1:E:262:ILE:HD11	1.63	0.80
1:F:161:VAL:HG11	1:G:134:VAL:HG12	1.64	0.80
1:E:137:ARG:HE	1:E:180:ASN:ND2	1.81	0.79
1:C:228:GLN:HG3	1:C:255:LEU:HB3	1.65	0.78
1:D:191:GLN:NE2	1:G:191:GLN:HE21	1.84	0.76
1:G:193:THR:HG22	2:G:395:HOH:O	1.84	0.76
1:D:23:VAL:HG11	1:D:55:ALA:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:VAL:HG12	1:E:161:VAL:HG11	1.67	0.75
1:D:191:GLN:NE2	1:G:191:GLN:NE2	2.35	0.75
1:F:17:ALA:HB1	1:F:70:VAL:HG12	1.69	0.75
1:F:23:VAL:HG11	1:F:55:ALA:HB2	1.69	0.75
1:C:193:THR:HG22	2:C:380:HOH:O	1.86	0.74
1:F:228:GLN:HG3	1:F:255:LEU:HB3	1.69	0.74
1:E:200:LYS:HZ2	1:G:124:THR:HG21	1.51	0.74
1:D:174:GLY:HA2	1:D:194:ILE:HD11	1.68	0.74
1:E:193:THR:HG22	2:E:385:HOH:O	1.87	0.73
1:F:337:LEU:CD2	1:F:363:PRO:HB2	2.19	0.72
1:A:200:LYS:HZ1	1:E:124:THR:HG21	1.52	0.72
1:E:23:VAL:HG11	1:E:55:ALA:HB2	1.71	0.72
1:D:122:ASP:OD1	1:D:124:THR:HG23	1.89	0.72
1:D:191:GLN:HE21	1:G:191:GLN:HE21	1.39	0.71
1:C:256:MET:HE3	1:C:291:VAL:HG11	1.73	0.71
1:D:26:LEU:HD13	1:D:320:LEU:HD12	1.73	0.70
1:A:62:GLU:HB2	2:A:404:HOH:O	1.92	0.70
1:F:111:THR:HB	1:F:343:HIS:CD2	2.28	0.69
1:A:124:THR:HG21	1:G:200:LYS:NZ	2.08	0.68
1:C:26:LEU:HD13	1:C:320:LEU:HD12	1.74	0.68
1:E:137:ARG:NE	1:E:180:ASN:HD22	1.88	0.68
1:G:137:ARG:HE	1:G:180:ASN:ND2	1.78	0.68
1:D:253:LEU:HD12	1:D:256:MET:HE2	1.76	0.68
1:D:314:GLN:O	1:D:317:PRO:HD2	1.92	0.68
1:E:200:LYS:NZ	1:G:124:THR:HG21	2.08	0.68
1:F:111:THR:HB	1:F:343:HIS:HD2	1.57	0.68
1:A:134:VAL:HG22	1:A:300:PRO:HG3	1.77	0.67
1:D:200:LYS:NZ	1:F:124:THR:HG21	2.08	0.67
1:G:29:ARG:HH11	1:G:29:ARG:HG3	1.59	0.67
1:F:174:GLY:HA2	1:F:194:ILE:HD11	1.77	0.67
1:D:256:MET:CE	1:D:262:ILE:HD11	2.24	0.67
1:A:191:GLN:HE22	1:C:191:GLN:NE2	1.92	0.67
1:E:191:GLN:HE21	1:F:191:GLN:NE2	1.93	0.67
1:A:145:GLN:NE2	2:A:426:HOH:O	2.28	0.66
1:D:200:LYS:HZ1	1:F:124:THR:HG21	1.60	0.66
1:C:47:ASP:HB3	1:C:57:LEU:HD13	1.78	0.66
1:G:122:ASP:OD1	1:G:124:THR:HG23	1.95	0.65
1:D:145:GLN:NE2	2:D:376:HOH:O	2.29	0.65
1:G:346:ARG:HG3	1:G:346:ARG:HH11	1.62	0.65
1:G:145:GLN:NE2	2:G:386:HOH:O	2.29	0.65
1:D:193:THR:HG22	2:D:388:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ARG:O	1:E:103:GLU:HG3	1.98	0.64
1:G:26:LEU:CD1	1:G:320:LEU:HD12	2.28	0.64
1:A:137:ARG:HE	1:A:180:ASN:ND2	1.87	0.64
1:E:18:LEU:HD12	2:E:393:HOH:O	1.97	0.64
1:F:134:VAL:HG12	1:G:161:VAL:HG11	1.80	0.63
1:F:256:MET:CE	1:F:262:ILE:HD11	2.28	0.63
1:E:256:MET:CE	1:E:262:ILE:HD11	2.28	0.63
1:D:99:ARG:O	1:D:103:GLU:HG3	1.98	0.63
1:G:119:GLN:HB2	1:G:125:LEU:HD23	1.80	0.63
1:F:93:LEU:HD12	1:F:114:ALA:HB2	1.80	0.63
1:C:145:GLN:NE2	2:C:431:HOH:O	2.31	0.63
1:E:117:THR:OG1	1:E:339:GLY:HA2	1.98	0.63
1:D:17:ALA:HB1	1:D:70:VAL:HG12	1.80	0.63
1:G:3:ILE:HD11	1:G:323:ALA:HB2	1.81	0.62
1:F:47:ASP:HB3	1:F:57:LEU:HD13	1.80	0.62
1:G:23:VAL:HG11	1:G:55:ALA:HB2	1.82	0.62
1:A:111:THR:HB	1:A:343:HIS:HD2	1.64	0.62
1:E:106:LEU:O	1:E:345:GLY:HA2	2.00	0.62
1:G:26:LEU:HD13	1:G:320:LEU:HD12	1.81	0.62
1:F:122:ASP:OD1	1:F:124:THR:HG23	2.00	0.62
1:D:228:GLN:HG3	1:D:255:LEU:HB3	1.81	0.62
1:E:294:TYR:CZ	1:E:296:VAL:HB	2.35	0.61
1:F:204:TYR:O	1:F:208:VAL:HG13	2.00	0.61
1:G:2:VAL:O	1:G:66:ALA:HB1	2.00	0.61
1:E:67:GLU:O	1:E:88:ILE:HG23	1.99	0.61
1:G:256:MET:CE	1:G:262:ILE:HD11	2.30	0.61
1:A:174:GLY:HA2	1:A:194:ILE:HD11	1.81	0.61
1:D:299:MET:N	1:D:300:PRO:CD	2.63	0.61
1:A:47:ASP:HB3	1:A:57:LEU:CD1	2.31	0.61
1:A:337:LEU:CD2	1:A:363:PRO:HB2	2.31	0.61
1:G:69:VAL:HG23	1:G:87:LEU:HD11	1.83	0.61
1:E:95:LEU:HD12	1:E:341:ASN:HD22	1.66	0.60
1:F:87:LEU:O	1:F:111:THR:HG23	2.01	0.60
1:G:294:TYR:CZ	1:G:296:VAL:HB	2.34	0.60
1:C:29:ARG:HG3	1:C:29:ARG:HH11	1.66	0.60
1:F:99:ARG:O	1:F:103:GLU:HG3	2.01	0.60
1:D:26:LEU:CD1	1:D:320:LEU:HD12	2.31	0.60
1:D:95:LEU:HD12	1:D:341:ASN:HD22	1.67	0.60
1:G:26:LEU:HD13	1:G:320:LEU:CD1	2.31	0.60
1:A:170:VAL:HG22	1:A:193:THR:CG2	2.31	0.60
1:C:111:THR:HA	1:C:342:THR:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HB3	1:A:95:LEU:CD2	2.32	0.60
1:E:191:GLN:NE2	1:F:191:GLN:NE2	2.49	0.60
1:C:157:LEU:HD21	1:E:137:ARG:HB2	1.84	0.60
1:E:122:ASP:OD1	1:E:124:THR:HG23	2.02	0.59
1:G:122:ASP:CG	1:G:124:THR:HG23	2.22	0.59
1:A:219:THR:O	1:A:223:ILE:HG13	2.02	0.59
1:A:294:TYR:CZ	1:A:296:VAL:HB	2.37	0.59
1:C:17:ALA:HB1	1:C:70:VAL:HG12	1.84	0.59
1:C:26:LEU:HD13	1:C:320:LEU:CD1	2.32	0.59
1:A:124:THR:HG21	1:G:200:LYS:HZ3	1.68	0.59
1:A:191:GLN:HE22	1:C:191:GLN:HE22	1.50	0.59
1:C:299:MET:N	1:C:300:PRO:CD	2.65	0.59
1:G:145:GLN:O	1:G:148:GLU:HB2	2.02	0.59
1:D:29:ARG:HG3	1:D:29:ARG:HH11	1.67	0.58
1:E:2:VAL:O	1:E:66:ALA:HB1	2.03	0.58
1:C:256:MET:CE	1:C:262:ILE:HD11	2.33	0.58
1:G:172:LEU:HD23	1:G:195:LEU:HD13	1.86	0.58
1:A:99:ARG:O	1:A:103:GLU:HG3	2.02	0.58
1:A:93:LEU:HB3	1:A:95:LEU:HD21	1.85	0.58
1:D:191:GLN:HE22	1:G:191:GLN:NE2	2.01	0.58
1:E:140:PRO:HG3	1:E:184:ILE:HB	1.85	0.58
1:E:29:ARG:HG3	1:E:29:ARG:HH11	1.68	0.58
1:E:142:VAL:HG21	1:E:299:MET:HE2	1.85	0.58
1:F:68:MET:HG3	1:F:88:ILE:HG13	1.84	0.58
1:F:209:PHE:O	1:F:212:ARG:HD3	2.03	0.58
1:A:249:THR:C	1:A:251:ASP:H	2.07	0.58
1:C:111:THR:HB	1:C:343:HIS:CD2	2.39	0.58
1:G:111:THR:HB	1:G:343:HIS:CD2	2.33	0.58
1:E:62:GLU:HB2	2:E:408:HOH:O	2.04	0.58
1:F:170:VAL:HG22	1:F:193:THR:HG23	1.85	0.57
1:E:87:LEU:O	1:E:111:THR:HG23	2.04	0.57
1:G:299:MET:N	1:G:300:PRO:CD	2.68	0.57
1:F:22:GLY:O	1:F:26:LEU:HD23	2.05	0.57
1:F:95:LEU:HD12	1:F:341:ASN:HB3	1.87	0.57
1:A:133:GLU:OE1	1:G:199:HIS:HE1	1.88	0.56
1:E:299:MET:N	1:E:300:PRO:CD	2.68	0.56
1:A:11:THR:O	1:A:12:LEU:HB2	2.04	0.56
1:A:194:ILE:HD13	1:A:205:LEU:HD13	1.87	0.56
1:A:288:VAL:HB	1:A:293:HIS:CE1	2.39	0.56
1:C:99:ARG:O	1:C:103:GLU:HG3	2.05	0.56
1:D:122:ASP:CG	1:D:124:THR:HG23	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:ARG:NE	1:F:180:ASN:HD22	1.91	0.56
1:F:337:LEU:HD22	1:F:363:PRO:HB2	1.88	0.56
1:G:99:ARG:O	1:G:103:GLU:HG3	2.04	0.56
1:E:117:THR:HG1	1:E:339:GLY:HA2	1.71	0.56
1:G:316:LEU:HB3	1:G:317:PRO:HD3	1.87	0.56
1:D:194:ILE:HD13	1:D:205:LEU:HD13	1.87	0.56
1:G:228:GLN:HG3	1:G:255:LEU:HB3	1.87	0.56
1:D:140:PRO:HG3	1:D:184:ILE:HB	1.88	0.56
1:D:47:ASP:HB3	1:D:57:LEU:HD13	1.86	0.56
1:A:348:THR:HA	1:A:361:THR:O	2.04	0.56
1:D:2:VAL:HG22	1:D:32:THR:HG23	1.88	0.55
1:E:47:ASP:HB3	1:E:57:LEU:HD13	1.88	0.55
1:E:316:LEU:HB3	1:E:317:PRO:HD3	1.88	0.55
1:F:170:VAL:HG22	1:F:193:THR:CG2	2.35	0.55
1:F:299:MET:N	1:F:300:PRO:CD	2.70	0.55
1:C:122:ASP:OD1	1:C:124:THR:HG23	2.06	0.55
1:D:69:VAL:HG23	1:D:87:LEU:HD11	1.89	0.55
1:E:99:ARG:HB2	1:E:356:PHE:CE1	2.42	0.55
1:C:111:THR:HB	1:C:343:HIS:HD2	1.71	0.55
1:E:253:LEU:HD12	1:E:256:MET:HE1	1.88	0.55
1:C:87:LEU:O	1:C:111:THR:HG23	2.07	0.55
1:C:200:LYS:NZ	1:D:124:THR:HG21	2.21	0.55
1:D:256:MET:HE1	1:D:291:VAL:HG11	1.89	0.55
1:C:174:GLY:HA2	1:C:194:ILE:HD11	1.90	0.54
1:C:142:VAL:HB	1:C:299:MET:HE1	1.88	0.54
1:E:47:ASP:HB3	1:E:57:LEU:CD1	2.38	0.54
1:A:23:VAL:HG11	1:A:55:ALA:HB2	1.89	0.54
1:A:87:LEU:O	1:A:111:THR:HG23	2.08	0.54
1:C:256:MET:HE3	1:C:262:ILE:HD11	1.90	0.54
1:E:134:VAL:CG2	1:E:300:PRO:HG3	2.37	0.54
1:F:193:THR:HG22	2:F:386:HOH:O	2.07	0.54
1:A:140:PRO:HG3	1:A:184:ILE:HB	1.90	0.54
1:D:158:LEU:HB3	1:D:190:ALA:HB2	1.88	0.54
1:E:204:TYR:O	1:E:208:VAL:HG13	2.08	0.54
1:A:299:MET:N	1:A:300:PRO:CD	2.71	0.53
1:D:231:ASP:OD1	1:D:257:LYS:HE3	2.08	0.53
1:F:288:VAL:O	1:F:289:ASP:HB2	2.08	0.53
1:A:26:LEU:HD13	1:A:320:LEU:HD12	1.91	0.53
1:A:26:LEU:HD13	1:A:320:LEU:CD1	2.38	0.53
1:A:337:LEU:HD22	1:A:363:PRO:HB2	1.90	0.53
1:C:3:ILE:HD12	1:C:26:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ILE:HG13	1:D:88:ILE:O	2.07	0.53
1:E:11:THR:O	1:E:12:LEU:HB2	2.07	0.53
1:E:170:VAL:HG22	1:E:193:THR:HG23	1.90	0.53
1:G:346:ARG:HG3	1:G:346:ARG:NH1	2.24	0.53
1:D:93:LEU:HB2	1:D:114:ALA:HB2	1.90	0.53
1:F:158:LEU:HB3	1:F:190:ALA:HB2	1.91	0.53
1:A:111:THR:HB	1:A:343:HIS:CD2	2.42	0.53
1:A:177:VAL:HB	1:A:236:ALA:HB1	1.89	0.53
1:C:26:LEU:CD1	1:C:320:LEU:HD12	2.38	0.53
1:F:316:LEU:HB3	1:F:317:PRO:HD3	1.90	0.53
1:E:8:GLU:HA	2:E:383:HOH:O	2.09	0.53
1:C:88:ILE:HG13	1:C:88:ILE:O	2.09	0.53
1:D:119:GLN:O	1:D:335:ALA:HA	2.09	0.53
1:E:202:LEU:HD12	2:E:424:HOH:O	2.09	0.53
1:C:161:VAL:HG11	1:E:134:VAL:HG12	1.89	0.53
1:G:343:HIS:CE1	1:G:367:LEU:HD12	2.44	0.53
1:A:294:TYR:OH	1:A:296:VAL:HB	2.09	0.53
1:E:26:LEU:HD13	1:E:320:LEU:HD12	1.92	0.52
1:G:29:ARG:HG3	1:G:29:ARG:NH1	2.22	0.52
1:G:299:MET:HB2	1:G:300:PRO:HD3	1.91	0.52
1:E:363:PRO:O	1:E:367:LEU:HB2	2.08	0.52
1:E:356:PHE:O	1:E:358:LEU:HG	2.09	0.52
1:A:161:VAL:HG11	1:D:134:VAL:HG12	1.91	0.52
1:C:71:LYS:HE3	1:C:73:LYS:O	2.10	0.52
1:A:47:ASP:HB3	1:A:57:LEU:HD13	1.92	0.52
1:E:142:VAL:HG21	1:E:299:MET:CE	2.38	0.52
1:A:256:MET:CE	1:A:262:ILE:HD11	2.39	0.52
1:E:106:LEU:HD11	1:E:347:LEU:HD13	1.92	0.52
1:F:256:MET:HE1	1:F:262:ILE:HD11	1.90	0.52
1:D:2:VAL:O	1:D:66:ALA:HB1	2.09	0.52
1:A:249:THR:C	1:A:251:ASP:N	2.63	0.51
1:G:88:ILE:O	1:G:88:ILE:HG13	2.10	0.51
1:C:23:VAL:HG22	1:C:33:VAL:HG11	1.92	0.51
1:C:137:ARG:HB2	1:E:157:LEU:HD21	1.92	0.51
1:D:92:TYR:CD1	1:D:115:TYR:HB2	2.44	0.51
1:E:134:VAL:HG22	1:E:300:PRO:HG3	1.92	0.51
1:F:145:GLN:NE2	2:F:433:HOH:O	2.43	0.51
1:F:26:LEU:HD13	1:F:320:LEU:HD12	1.92	0.51
1:F:337:LEU:HD21	1:F:363:PRO:HB2	1.91	0.51
1:A:350:PRO:HD3	1:A:360:TYR:CE1	2.46	0.51
1:E:16:VAL:HG22	1:E:18:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:348:THR:HA	1:G:361:THR:O	2.11	0.51
1:C:253:LEU:HD12	1:C:256:MET:HE1	1.93	0.51
1:D:26:LEU:HD13	1:D:320:LEU:CD1	2.41	0.51
1:D:139:ALA:HB1	1:D:234:ILE:HD13	1.93	0.51
1:C:149:LYS:HB3	1:C:150:PRO:HD3	1.92	0.51
1:A:232:LEU:HD13	1:A:261:VAL:HG22	1.93	0.50
1:D:149:LYS:HB3	1:D:150:PRO:HD3	1.92	0.50
1:E:111:THR:HB	1:E:343:HIS:CD2	2.35	0.50
1:C:142:VAL:HG11	1:C:294:TYR:CE2	2.45	0.50
1:D:120:LEU:HD12	1:D:124:THR:OG1	2.11	0.50
1:A:35:VAL:HG23	1:A:55:ALA:HB1	1.94	0.50
1:E:191:GLN:NE2	1:F:191:GLN:HE22	2.09	0.50
1:G:256:MET:HE1	1:G:262:ILE:HD11	1.92	0.50
1:C:288:VAL:O	1:C:289:ASP:HB2	2.12	0.50
1:G:170:VAL:HG21	1:G:226:SER:O	2.12	0.50
1:E:288:VAL:O	1:E:289:ASP:HB2	2.12	0.50
1:D:288:VAL:HB	1:D:293:HIS:CE1	2.47	0.50
1:D:294:TYR:CZ	1:D:296:VAL:HB	2.47	0.50
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.27	0.50
1:E:93:LEU:HD12	1:E:114:ALA:HB2	1.94	0.50
1:D:299:MET:HB2	1:D:300:PRO:HD3	1.94	0.50
1:F:24:GLU:O	1:F:28:ARG:HB2	2.12	0.49
1:C:170:VAL:HG22	1:C:193:THR:CG2	2.42	0.49
1:F:250:ARG:HA	1:F:253:LEU:HB2	1.94	0.49
1:C:47:ASP:HB3	1:C:57:LEU:CD1	2.41	0.49
1:D:142:VAL:HG21	1:D:299:MET:HE2	1.93	0.49
1:E:104:ALA:HA	1:E:107:ARG:NH1	2.27	0.49
1:G:116:GLU:HG2	1:G:117:THR:HG23	1.95	0.49
1:A:288:VAL:O	1:A:289:ASP:HB2	2.12	0.49
1:G:288:VAL:O	1:G:289:ASP:HB2	2.12	0.49
1:A:67:GLU:O	1:A:87:LEU:HD12	2.12	0.49
1:A:124:THR:HG21	1:G:200:LYS:HZ1	1.77	0.49
1:C:199:HIS:HD2	2:C:371:HOH:O	1.94	0.49
1:D:11:THR:O	1:D:12:LEU:HB2	2.13	0.49
1:A:19:THR:O	1:A:20:PRO:C	2.49	0.49
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.78	0.49
1:C:29:ARG:HG3	1:C:29:ARG:NH1	2.27	0.49
1:C:314:GLN:O	1:C:317:PRO:HD2	2.13	0.49
1:D:29:ARG:HG3	1:D:29:ARG:NH1	2.25	0.49
1:C:117:THR:OG1	1:C:339:GLY:HA2	2.13	0.49
1:E:358:LEU:HB3	1:E:359:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:THR:OG1	1:G:339:GLY:HA2	2.13	0.49
1:A:206:ASP:O	1:A:210:GLY:O	2.31	0.48
1:G:87:LEU:O	1:G:110:VAL:HG23	2.13	0.48
1:G:125:LEU:HD12	1:G:128:LEU:HD23	1.95	0.48
1:F:137:ARG:HB2	1:G:157:LEU:HD21	1.95	0.48
1:G:263:VAL:HG11	1:G:299:MET:HE3	1.95	0.48
1:E:179:THR:O	1:E:182:ALA:HB3	2.13	0.48
1:F:2:VAL:O	1:F:66:ALA:HB1	2.14	0.48
1:A:301:GLY:O	1:A:304:PRO:HD3	2.13	0.48
1:F:34:LEU:HD12	1:F:56:GLU:HB2	1.95	0.48
1:G:111:THR:HA	1:G:342:THR:O	2.14	0.48
1:F:130:PRO:HG3	1:F:314:GLN:HG3	1.96	0.48
1:G:93:LEU:HD12	1:G:114:ALA:HB2	1.95	0.48
1:G:294:TYR:OH	1:G:296:VAL:HB	2.13	0.48
1:A:95:LEU:HB2	1:A:352:VAL:HG21	1.96	0.48
1:F:1:MET:N	1:F:31:HIS:HD2	2.12	0.48
1:A:169:VAL:HG22	1:A:232:LEU:HB3	1.95	0.48
1:A:256:MET:CE	1:A:291:VAL:HG11	2.32	0.48
1:C:204:TYR:O	1:C:208:VAL:HG13	2.11	0.48
1:C:287:VAL:HG13	1:C:291:VAL:O	2.14	0.48
1:G:149:LYS:HB3	1:G:150:PRO:HD3	1.94	0.48
1:A:68:MET:HA	1:A:88:ILE:HG23	1.95	0.48
1:A:200:LYS:HZ2	1:E:124:THR:HG21	1.74	0.48
1:F:353:ALA:CB	1:F:360:TYR:HB2	2.43	0.48
1:E:362:PRO:HB2	1:E:365:GLU:HB2	1.96	0.47
1:F:197:VAL:O	1:F:197:VAL:HG12	2.13	0.47
1:G:102:THR:O	1:G:106:LEU:HG	2.13	0.47
1:A:47:ASP:HB3	1:A:57:LEU:HD11	1.96	0.47
1:C:127:LEU:HD22	1:C:315:THR:HG22	1.96	0.47
1:G:253:LEU:HD12	1:G:256:MET:HE1	1.96	0.47
1:A:67:GLU:O	1:A:88:ILE:HG23	2.14	0.47
1:E:209:PHE:O	1:E:212:ARG:HD3	2.14	0.47
1:D:72:VAL:O	1:D:92:TYR:HB2	2.14	0.47
1:E:17:ALA:HB1	1:E:70:VAL:HG12	1.96	0.47
1:E:103:GLU:O	1:E:107:ARG:HG3	2.15	0.47
1:E:362:PRO:HB2	1:E:365:GLU:CB	2.44	0.47
1:F:253:LEU:HD12	1:F:256:MET:HE1	1.96	0.47
1:D:2:VAL:HG22	1:D:32:THR:CG2	2.45	0.47
1:E:253:LEU:HD12	1:E:256:MET:CE	2.44	0.47
1:G:350:PRO:HD3	1:G:360:TYR:CE1	2.49	0.47
1:C:23:VAL:HG11	1:C:55:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:VAL:HG21	1:E:300:PRO:HB3	1.96	0.47
1:C:11:THR:O	1:C:12:LEU:HB2	2.15	0.46
1:A:316:LEU:HB3	1:A:317:PRO:HD3	1.97	0.46
1:D:253:LEU:HD12	1:D:256:MET:CE	2.42	0.46
1:A:224:LYS:NZ	1:E:28:ARG:HH12	2.14	0.46
1:C:209:PHE:O	1:C:212:ARG:HD3	2.15	0.46
1:C:248:VAL:HA	1:C:252:MET:SD	2.55	0.46
1:D:22:GLY:O	1:D:26:LEU:HD22	2.16	0.46
1:D:106:LEU:O	1:D:345:GLY:HA2	2.15	0.46
1:D:145:GLN:O	1:D:148:GLU:HB2	2.14	0.46
1:A:68:MET:HA	1:A:88:ILE:O	2.16	0.46
1:A:204:TYR:O	1:A:208:VAL:HG13	2.16	0.46
1:A:204:TYR:O	1:A:208:VAL:CG1	2.64	0.46
1:C:200:LYS:HZ1	1:D:124:THR:HG21	1.79	0.46
1:F:1:MET:HG2	1:F:2:VAL:N	2.31	0.46
1:F:95:LEU:CD1	1:F:341:ASN:HB3	2.46	0.46
1:D:111:THR:HB	1:D:343:HIS:CD2	2.51	0.46
1:D:138:MET:O	1:D:141:GLN:HB3	2.16	0.46
1:E:60:ARG:NH1	1:E:60:ARG:HG3	2.30	0.46
1:A:170:VAL:HG22	1:A:193:THR:HG21	1.97	0.46
1:A:235:GLY:O	1:A:265:VAL:HG23	2.16	0.46
1:F:142:VAL:HG21	1:F:299:MET:CE	2.46	0.46
1:F:186:LEU:HG	1:F:213:VAL:HG23	1.98	0.46
1:G:99:ARG:HD2	1:G:356:PHE:CD1	2.51	0.46
1:A:26:LEU:CD1	1:A:320:LEU:HD12	2.47	0.45
1:A:71:LYS:HE3	1:A:73:LYS:O	2.16	0.45
1:C:119:GLN:O	1:C:335:ALA:HA	2.16	0.45
1:C:337:LEU:CD2	1:C:363:PRO:HB2	2.46	0.45
1:D:129:VAL:N	1:D:130:PRO:CD	2.79	0.45
1:D:301:GLY:O	1:D:304:PRO:HD3	2.16	0.45
1:A:248:VAL:HA	1:A:252:MET:SD	2.56	0.45
1:C:346:ARG:HH11	1:C:346:ARG:HG3	1.81	0.45
1:D:137:ARG:NE	1:D:180:ASN:HD22	1.97	0.45
1:E:93:LEU:O	1:E:94:HIS:C	2.55	0.45
1:E:125:LEU:O	1:E:129:VAL:HG23	2.16	0.45
1:F:11:THR:O	1:F:12:LEU:HB2	2.16	0.45
1:D:237:VAL:HB	1:D:238:LEU:H	1.57	0.45
1:D:263:VAL:HG11	1:D:299:MET:HE3	1.99	0.45
1:A:134:VAL:CG2	1:A:300:PRO:HG3	2.44	0.45
1:E:223:ILE:O	1:E:227:VAL:HG23	2.17	0.45
1:D:195:LEU:HG	1:D:216:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:LYS:HB3	1:E:150:PRO:HD3	1.98	0.45
1:F:49:GLU:HA	1:F:52:ARG:NH1	2.32	0.45
1:A:228:GLN:HG3	1:A:255:LEU:HB3	1.98	0.45
1:A:299:MET:HB2	1:A:300:PRO:HD3	1.99	0.45
1:A:130:PRO:CG	1:A:314:GLN:HG3	2.47	0.45
1:C:147:LEU:HD12	1:C:158:LEU:HD21	1.98	0.45
1:D:134:VAL:HG21	1:D:300:PRO:HB3	1.99	0.45
1:A:157:LEU:HD21	1:D:137:ARG:HB2	1.98	0.45
1:E:130:PRO:HG2	1:E:314:GLN:HG3	1.99	0.45
1:A:88:ILE:O	1:A:88:ILE:HG13	2.16	0.44
1:D:137:ARG:HE	1:D:180:ASN:ND2	1.97	0.44
1:C:256:MET:HE1	1:C:262:ILE:HD11	1.99	0.44
1:C:337:LEU:HD22	1:C:363:PRO:HB2	2.00	0.44
1:E:9:ILE:CD1	1:E:76:LEU:HD12	2.47	0.44
1:E:129:VAL:HB	1:E:130:PRO:HD3	1.98	0.44
1:E:174:GLY:HA2	1:E:194:ILE:HD11	2.00	0.44
1:E:294:TYR:OH	1:E:296:VAL:HB	2.16	0.44
1:A:256:MET:HE3	1:A:262:ILE:HD11	2.00	0.44
1:F:29:ARG:HG3	1:F:29:ARG:HH11	1.81	0.44
1:E:299:MET:HB2	1:E:300:PRO:HD3	1.99	0.44
1:G:104:ALA:HA	1:G:107:ARG:NH1	2.32	0.44
1:G:170:VAL:HG22	1:G:193:THR:HG23	1.98	0.44
1:D:195:LEU:HA	1:D:216:LEU:O	2.18	0.44
1:D:264:ASP:OD1	1:D:266:ALA:HB3	2.18	0.44
1:C:223:ILE:O	1:C:227:VAL:HG23	2.18	0.44
1:C:330:LEU:HD12	1:C:330:LEU:N	2.33	0.44
1:F:149:LYS:HB3	1:F:150:PRO:HD3	2.00	0.44
1:C:72:VAL:O	1:C:92:TYR:HB2	2.18	0.43
1:E:205:LEU:HD23	1:E:205:LEU:HA	1.87	0.43
1:F:71:LYS:HE3	1:F:73:LYS:O	2.17	0.43
1:G:61:GLU:CD	1:G:61:GLU:H	2.21	0.43
1:G:95:LEU:HD12	1:G:341:ASN:HD22	1.83	0.43
1:A:223:ILE:O	1:A:227:VAL:HG23	2.18	0.43
1:C:170:VAL:HG11	1:C:226:SER:HB3	2.00	0.43
1:F:77:PRO:HA	1:F:80:TYR:CE2	2.53	0.43
1:G:91:THR:HA	1:G:115:TYR:CE2	2.53	0.43
1:D:125:LEU:O	1:D:129:VAL:HG23	2.18	0.43
1:E:298:ASN:HD22	1:E:301:GLY:HA3	1.83	0.43
1:G:11:THR:O	1:G:12:LEU:HB2	2.18	0.43
1:C:322:LEU:HD21	1:C:330:LEU:HD11	2.00	0.43
1:D:134:VAL:HG23	1:D:300:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:GLU:HA	1:G:52:ARG:NH1	2.34	0.43
1:A:28:ARG:HH12	1:G:224:LYS:NZ	2.16	0.43
1:E:110:VAL:HG22	1:E:111:THR:N	2.34	0.43
1:E:342:THR:HA	1:E:346:ARG:O	2.19	0.43
1:D:95:LEU:CD1	1:D:341:ASN:HD22	2.31	0.43
1:D:340:LEU:HG	1:D:348:THR:OG1	2.17	0.43
1:C:49:GLU:HA	1:C:52:ARG:NH1	2.34	0.43
1:D:194:ILE:HD13	1:D:205:LEU:CD1	2.48	0.43
1:E:105:MET:CE	1:E:112:GLY:HA3	2.49	0.43
1:E:199:HIS:HD2	2:E:424:HOH:O	2.01	0.43
1:F:88:ILE:HG13	1:F:88:ILE:O	2.19	0.43
1:A:249:THR:OG1	1:A:251:ASP:HB2	2.18	0.43
1:A:16:VAL:HG11	1:A:45:LEU:HD12	2.00	0.43
1:A:222:ASN:HD22	1:A:222:ASN:HA	1.60	0.43
1:E:37:ARG:NH2	2:E:403:HOH:O	2.52	0.43
1:E:50:TYR:O	1:E:53:ALA:HB3	2.19	0.43
1:E:99:ARG:HD2	1:E:356:PHE:CD1	2.54	0.43
1:F:195:LEU:HG	1:F:216:LEU:HB2	2.01	0.43
1:C:350:PRO:HD3	1:C:360:TYR:CE1	2.54	0.43
1:E:298:ASN:ND2	1:E:301:GLY:CA	2.82	0.43
1:F:363:PRO:O	1:F:367:LEU:HB2	2.19	0.42
1:G:99:ARG:HB2	1:G:356:PHE:CE1	2.54	0.42
1:A:129:VAL:HB	1:A:130:PRO:HD3	2.01	0.42
1:E:250:ARG:HG2	1:E:250:ARG:HH11	1.84	0.42
1:F:1:MET:N	1:F:31:HIS:CD2	2.87	0.42
1:G:106:LEU:HD23	1:G:106:LEU:HA	1.84	0.42
1:G:122:ASP:OD2	1:G:124:THR:HG23	2.19	0.42
1:A:308:THR:O	1:A:312:THR:HG23	2.19	0.42
1:D:23:VAL:HG22	1:D:33:VAL:HG11	2.01	0.42
1:F:301:GLY:O	1:F:304:PRO:HD3	2.19	0.42
1:A:177:VAL:HG23	2:A:398:HOH:O	2.18	0.42
1:C:84:ARG:HG2	1:C:84:ARG:HH11	1.84	0.42
1:C:170:VAL:HG22	1:C:193:THR:HG23	2.00	0.42
1:F:34:LEU:HD11	2:F:375:HOH:O	2.18	0.42
1:F:142:VAL:HG11	1:F:294:TYR:CE2	2.54	0.42
1:A:35:VAL:CG2	1:A:55:ALA:HB1	2.50	0.42
1:D:142:VAL:HG21	1:D:299:MET:CE	2.50	0.42
1:F:349:HIS:HA	1:F:350:PRO:HD2	1.82	0.42
1:C:204:TYR:CE2	1:C:208:VAL:HG11	2.55	0.42
1:D:71:LYS:NZ	2:D:386:HOH:O	2.41	0.42
1:E:250:ARG:HG2	1:E:250:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:PRO:CG	1:F:314:GLN:HG3	2.49	0.42
1:D:163:GLY:O	1:G:216:LEU:HA	2.19	0.42
1:D:206:ASP:O	1:D:210:GLY:O	2.37	0.42
1:E:145:GLN:O	1:E:148:GLU:HB2	2.19	0.42
1:E:343:HIS:O	1:E:344:LYS:HB2	2.20	0.42
1:F:256:MET:HE3	1:F:262:ILE:HD11	2.02	0.42
1:A:1:MET:HG2	1:A:2:VAL:N	2.35	0.42
1:C:124:THR:HG21	1:F:200:LYS:HZ3	1.82	0.42
1:D:47:ASP:HB3	1:D:57:LEU:CD1	2.48	0.42
1:D:238:LEU:CB	1:D:266:ALA:HB1	2.49	0.42
1:E:130:PRO:CG	1:E:314:GLN:HG3	2.50	0.42
1:D:142:VAL:HG11	1:D:294:TYR:CE2	2.55	0.42
1:D:316:LEU:HB3	1:D:317:PRO:HD3	2.00	0.42
1:F:237:VAL:HB	1:F:238:LEU:H	1.51	0.42
1:G:209:PHE:O	1:G:212:ARG:HD3	2.20	0.42
1:A:9:ILE:HG13	1:A:76:LEU:HD12	2.02	0.41
1:C:38:GLY:HA2	1:C:41:GLU:HG3	2.02	0.41
1:F:350:PRO:HD3	1:F:360:TYR:CE1	2.55	0.41
1:A:92:TYR:CD1	1:A:115:TYR:HB2	2.55	0.41
1:A:173:GLY:O	1:A:178:GLY:HA3	2.20	0.41
1:D:288:VAL:O	1:D:289:ASP:HB2	2.20	0.41
1:D:77:PRO:HD2	2:D:390:HOH:O	2.19	0.41
1:E:172:LEU:HD23	1:E:195:LEU:HD13	2.01	0.41
1:E:320:LEU:HD12	1:E:320:LEU:HA	1.87	0.41
1:G:3:ILE:HD11	1:G:323:ALA:CB	2.47	0.41
1:G:114:ALA:N	1:G:339:GLY:O	2.48	0.41
1:A:256:MET:HE1	1:A:262:ILE:HD11	2.03	0.41
1:G:136:GLY:O	1:G:140:PRO:HD2	2.19	0.41
1:A:68:MET:CA	1:A:88:ILE:HG23	2.50	0.41
1:C:7:LYS:HG3	1:C:39:ALA:HA	2.03	0.41
1:E:1:MET:N	1:E:31:HIS:HD2	2.19	0.41
1:E:29:ARG:HG3	1:E:29:ARG:NH1	2.31	0.41
1:F:56:GLU:OE1	2:F:375:HOH:O	2.21	0.41
1:F:119:GLN:O	1:F:335:ALA:HA	2.21	0.41
1:G:288:VAL:HB	1:G:293:HIS:CE1	2.56	0.41
1:A:93:LEU:O	1:A:94:HIS:C	2.59	0.41
1:A:138:MET:SD	1:D:157:LEU:HD13	2.60	0.41
1:A:227:VAL:O	1:A:256:MET:HG2	2.20	0.41
1:A:349:HIS:HA	1:A:350:PRO:HD2	1.86	0.41
1:E:1:MET:HG3	1:E:67:GLU:OE1	2.21	0.41
1:E:75:PRO:HA	1:E:79:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:VAL:O	1:G:92:TYR:HB2	2.21	0.41
1:C:172:LEU:O	1:C:237:VAL:HG22	2.20	0.41
1:C:250:ARG:HH11	1:C:250:ARG:HG2	1.85	0.41
1:A:28:ARG:HH12	1:G:224:LYS:HZ2	1.69	0.41
1:C:122:ASP:CG	1:C:124:THR:HG23	2.41	0.41
1:C:237:VAL:HB	1:C:238:LEU:H	1.49	0.41
1:D:62:GLU:HB2	2:D:414:HOH:O	2.19	0.41
1:E:129:VAL:N	1:E:130:PRO:CD	2.84	0.41
1:E:348:THR:HA	1:E:361:THR:O	2.19	0.41
1:G:325:LYS:O	1:G:328:ASP:HB2	2.21	0.41
1:G:367:LEU:HD12	1:G:367:LEU:HA	1.84	0.41
1:A:142:VAL:HG21	1:A:299:MET:CE	2.50	0.41
1:A:224:LYS:NZ	1:E:28:ARG:NH1	2.68	0.41
1:A:315:THR:O	1:A:319:VAL:HG23	2.21	0.41
1:C:95:LEU:HD12	1:C:341:ASN:HB3	2.03	0.41
1:C:140:PRO:HG3	1:C:184:ILE:HB	2.03	0.41
1:D:337:LEU:CD2	1:D:363:PRO:HB2	2.51	0.41
1:E:61:GLU:HG3	1:E:82:PHE:HE2	1.86	0.41
1:F:26:LEU:CD1	1:F:320:LEU:HD12	2.51	0.41
1:F:129:VAL:N	1:F:130:PRO:CD	2.84	0.41
1:A:130:PRO:HG3	1:A:314:GLN:HG3	2.02	0.41
1:C:69:VAL:HG23	1:C:87:LEU:HD11	2.03	0.41
1:D:68:MET:HG3	1:D:88:ILE:HG13	2.03	0.41
1:E:78:GLU:HB3	2:E:387:HOH:O	2.20	0.41
1:A:3:ILE:HD12	1:A:26:LEU:HG	2.02	0.40
1:A:142:VAL:HG21	1:A:299:MET:HE3	2.02	0.40
1:C:91:THR:HA	1:C:115:TYR:CE2	2.56	0.40
1:C:145:GLN:O	1:C:148:GLU:HB2	2.21	0.40
1:E:88:ILE:O	1:E:88:ILE:HG13	2.21	0.40
1:E:95:LEU:O	1:E:356:PHE:HE2	2.04	0.40
1:E:105:MET:HE1	1:E:112:GLY:HA3	2.03	0.40
1:F:134:VAL:HG21	1:F:300:PRO:HB3	2.04	0.40
1:D:204:TYR:O	1:D:208:VAL:HG13	2.21	0.40
1:A:60:ARG:CG	1:A:60:ARG:HH11	2.34	0.40
1:D:367:LEU:HD12	1:D:367:LEU:HA	1.88	0.40
1:E:165:ALA:HB2	1:F:216:LEU:HD21	2.03	0.40
1:F:199:HIS:O	1:F:203:GLN:HG3	2.21	0.40
1:F:232:LEU:HD13	1:F:261:VAL:HG22	2.03	0.40
1:A:193:THR:HG22	2:A:377:HOH:O	2.20	0.40
1:C:113:ILE:HA	1:C:339:GLY:O	2.22	0.40
1:D:224:LYS:HE2	1:D:224:LYS:HB2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LEU:HD12	1:E:124:THR:OG1	2.21	0.40
1:F:186:LEU:HG	1:F:213:VAL:CG2	2.52	0.40
1:G:84:ARG:O	1:G:110:VAL:HA	2.22	0.40
1:D:114:ALA:HB1	1:D:116:GLU:CD	2.42	0.40
1:F:2:VAL:HG22	1:F:32:THR:HG23	2.04	0.40
1:F:303:VAL:O	1:F:303:VAL:HG23	2.22	0.40
1:F:362:PRO:HA	1:F:363:PRO:HD2	1.87	0.40
1:G:219:THR:O	1:G:223:ILE:HG13	2.22	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	337/369 (91%)	308 (91%)	26 (8%)	3 (1%)	17	38
1	C	337/369 (91%)	319 (95%)	15 (4%)	3 (1%)	17	38
1	D	337/369 (91%)	317 (94%)	17 (5%)	3 (1%)	17	38
1	E	337/369 (91%)	310 (92%)	22 (6%)	5 (2%)	10	24
1	F	337/369 (91%)	317 (94%)	17 (5%)	3 (1%)	17	38
1	G	337/369 (91%)	324 (96%)	10 (3%)	3 (1%)	17	38
All	All	2022/2214 (91%)	1895 (94%)	107 (5%)	20 (1%)	15	35

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	VAL
1	A	297	ALA
1	C	297	ALA
1	D	297	ALA

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Mol	Chain	Res	Type
1	E	297	ALA
1	F	297	ALA
1	G	297	ALA
1	A	298	ASN
1	D	298	ASN
1	E	237	VAL
1	F	237	VAL
1	G	237	VAL
1	C	237	VAL
1	D	237	VAL
1	G	218	ALA
1	E	298	ASN
1	F	211	GLY
1	E	80	TYR
1	C	211	GLY
1	E	211	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	259/282 (92%)	244 (94%)	15 (6%)	20	42
1	C	259/282 (92%)	243 (94%)	16 (6%)	18	39
1	D	259/282 (92%)	248 (96%)	11 (4%)	30	56
1	E	259/282 (92%)	245 (95%)	14 (5%)	22	45
1	F	259/282 (92%)	246 (95%)	13 (5%)	24	49
1	G	259/282 (92%)	245 (95%)	14 (5%)	22	45
All	All	1554/1692 (92%)	1471 (95%)	83 (5%)	22	46

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	THR

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Mol	Chain	Res	Type
1	A	34	LEU
1	A	60	ARG
1	A	88	ILE
1	A	103	GLU
1	A	111	THR
1	A	134	VAL
1	A	161	VAL
1	A	186	LEU
1	A	237	VAL
1	A	253	LEU
1	A	261	VAL
1	A	320	LEU
1	A	337	LEU
1	C	26	LEU
1	C	32	THR
1	C	34	LEU
1	C	60	ARG
1	C	88	ILE
1	C	111	THR
1	C	134	VAL
1	C	186	LEU
1	C	193	THR
1	C	208	VAL
1	C	237	VAL
1	C	257	LYS
1	C	261	VAL
1	C	320	LEU
1	C	337	LEU
1	C	367	LEU
1	D	32	THR
1	D	60	ARG
1	D	88	ILE
1	D	111	THR
1	D	186	LEU
1	D	193	THR
1	D	222	ASN
1	D	237	VAL
1	D	305	ARG
1	D	320	LEU
1	D	337	LEU
1	E	32	THR
1	E	34	LEU

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Mol	Chain	Res	Type
1	E	60	ARG
1	E	74	GLU
1	E	88	ILE
1	E	90	PHE
1	E	111	THR
1	E	134	VAL
1	E	186	LEU
1	E	193	THR
1	E	237	VAL
1	E	305	ARG
1	E	320	LEU
1	E	337	LEU
1	F	32	THR
1	F	34	LEU
1	F	60	ARG
1	F	88	ILE
1	F	111	THR
1	F	186	LEU
1	F	193	THR
1	F	208	VAL
1	F	237	VAL
1	F	257	LYS
1	F	320	LEU
1	F	337	LEU
1	F	367	LEU
1	G	26	LEU
1	G	32	THR
1	G	34	LEU
1	G	60	ARG
1	G	74	GLU
1	G	88	ILE
1	G	111	THR
1	G	134	VAL
1	G	186	LEU
1	G	193	THR
1	G	237	VAL
1	G	261	VAL
1	G	320	LEU
1	G	337	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	31	HIS
1	A	141	GLN
1	A	145	GLN
1	A	180	ASN
1	A	191	GLN
1	A	199	HIS
1	A	222	ASN
1	A	343	HIS
1	C	14	ASN
1	C	31	HIS
1	C	141	GLN
1	C	180	ASN
1	C	199	HIS
1	C	222	ASN
1	C	298	ASN
1	C	341	ASN
1	C	343	HIS
1	D	14	ASN
1	D	31	HIS
1	D	119	GLN
1	D	141	GLN
1	D	180	ASN
1	D	191	GLN
1	D	199	HIS
1	D	222	ASN
1	D	293	HIS
1	D	341	ASN
1	D	343	HIS
1	E	31	HIS
1	E	141	GLN
1	E	145	GLN
1	E	180	ASN
1	E	199	HIS
1	E	222	ASN
1	E	298	ASN
1	E	341	ASN
1	E	343	HIS
1	F	31	HIS
1	F	141	GLN
1	F	145	GLN
1	F	180	ASN
1	F	191	GLN

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Mol	Chain	Res	Type
1	F	199	HIS
1	F	222	ASN
1	F	343	HIS
1	G	14	ASN
1	G	31	HIS
1	G	141	GLN
1	G	145	GLN
1	G	180	ASN
1	G	199	HIS
1	G	222	ASN
1	G	343	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	343/369 (92%)	0.20	28 (8%)	11	10	13, 35, 61, 72	0
1	C	343/369 (92%)	-0.01	19 (5%)	25	24	11, 26, 58, 70	0
1	D	343/369 (92%)	0.00	16 (4%)	31	30	15, 28, 59, 69	0
1	E	343/369 (92%)	0.09	23 (6%)	17	16	13, 34, 60, 72	0
1	F	343/369 (92%)	0.11	25 (7%)	15	13	11, 28, 60, 74	0
1	G	343/369 (92%)	-0.01	13 (3%)	40	40	14, 32, 59, 72	0
All	All	2058/2214 (92%)	0.06	124 (6%)	21	21	11, 31, 60, 74	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	ASP	6.3
1	D	238	LEU	6.2
1	F	368	ARG	5.9
1	G	369	GLY	5.7
1	F	369	GLY	5.5
1	F	289	ASP	5.1
1	A	369	GLY	4.8
1	A	238	LEU	4.7
1	F	297	ALA	4.7
1	F	288	VAL	4.5
1	C	252	MET	4.5
1	C	297	ALA	4.4
1	F	293	HIS	4.3
1	D	287	VAL	4.2
1	F	294	TYR	4.2
1	A	360	TYR	4.1
1	C	288	VAL	4.0
1	E	288	VAL	3.9
1	D	289	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	288	VAL	3.9
1	D	288	VAL	3.7
1	A	348	THR	3.7
1	C	251	ASP	3.6
1	A	346	ARG	3.6
1	A	250	ARG	3.6
1	F	331	LEU	3.6
1	C	287	VAL	3.6
1	A	287	VAL	3.5
1	E	369	GLY	3.5
1	A	361	THR	3.4
1	F	255	LEU	3.4
1	F	346	ARG	3.4
1	F	367	LEU	3.3
1	E	360	TYR	3.3
1	C	238	LEU	3.3
1	G	288	VAL	3.2
1	D	369	GLY	3.2
1	F	250	ARG	3.2
1	E	289	ASP	3.2
1	E	103	GLU	3.2
1	F	238	LEU	3.2
1	F	286	TYR	3.2
1	A	289	ASP	3.1
1	F	251	ASP	3.1
1	A	366	ALA	3.1
1	A	345	GLY	3.1
1	C	266	ALA	3.1
1	E	347	LEU	3.1
1	D	286	TYR	3.0
1	A	356	PHE	3.0
1	C	250	ARG	2.9
1	A	105	MET	2.9
1	C	294	TYR	2.9
1	D	297	ALA	2.9
1	E	367	LEU	2.9
1	G	356	PHE	2.8
1	A	359	PRO	2.8
1	F	266	ALA	2.8
1	F	287	VAL	2.8
1	A	368	ARG	2.8
1	E	356	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	346	ARG	2.8
1	F	364	GLU	2.8
1	G	110	VAL	2.7
1	A	293	HIS	2.7
1	A	344	LYS	2.7
1	E	348	THR	2.7
1	C	253	LEU	2.7
1	C	249	THR	2.7
1	E	362	PRO	2.6
1	D	293	HIS	2.6
1	E	361	THR	2.6
1	D	250	ARG	2.6
1	E	351	GLY	2.5
1	G	238	LEU	2.5
1	G	108	SER	2.5
1	G	289	ASP	2.5
1	E	357	GLY	2.4
1	F	365	GLU	2.4
1	F	295	GLY	2.4
1	E	101	LEU	2.4
1	A	106	LEU	2.4
1	F	247	LEU	2.4
1	A	343	HIS	2.4
1	F	249	THR	2.4
1	F	290	GLY	2.4
1	D	255	LEU	2.3
1	D	251	ASP	2.3
1	A	358	LEU	2.3
1	E	107	ARG	2.3
1	C	248	VAL	2.3
1	E	365	GLU	2.3
1	E	296	VAL	2.3
1	G	363	PRO	2.3
1	A	362	PRO	2.3
1	C	254	SER	2.2
1	D	364	GLU	2.2
1	F	252	MET	2.2
1	C	290	GLY	2.2
1	A	331	LEU	2.2
1	E	250	ARG	2.2
1	C	366	ALA	2.2
1	A	347	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	369	GLY	2.2
1	A	294	TYR	2.2
1	D	290	GLY	2.2
1	E	355	ALA	2.2
1	G	85	GLU	2.2
1	G	287	VAL	2.1
1	E	353	ALA	2.1
1	E	80	TYR	2.1
1	G	107	ARG	2.1
1	A	248	VAL	2.1
1	D	294	TYR	2.1
1	C	293	HIS	2.1
1	G	293	HIS	2.1
1	A	365	GLU	2.1
1	D	295	GLY	2.1
1	F	254	SER	2.1
1	G	251	ASP	2.1
1	D	107	ARG	2.1
1	A	349	HIS	2.1
1	E	354	GLU	2.0
1	C	295	GLY	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.