Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 11:15 PM JST

PDB ID	:	5YIT
Title	:	Crystal Structure of Hypothetical protein (Rv3272) from Mycobacterium tuberculosis
Authors	:	Karade, S.S.; Pratap, J.V.
Deposited on	:	2017-10-06
Resolution	:	2.79 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:

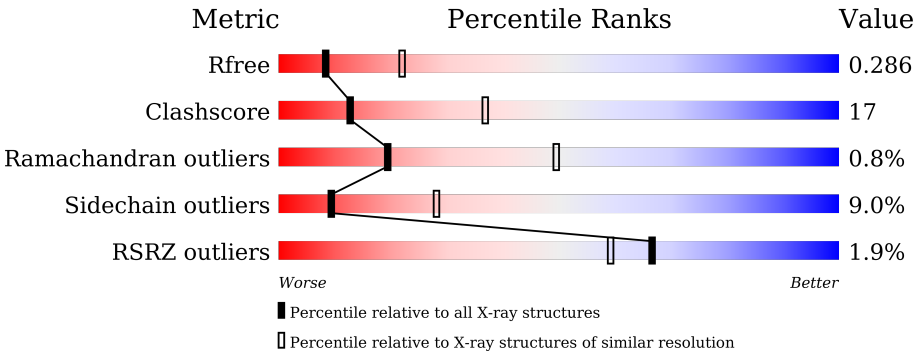
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	394	2% 64% 21% • 11%
1	B	394	% 72% 15% • 10%
1	C	394	2% 60% 26% • 10%
1	D	394	2% 65% 21% • 11%
1	E	394	2% 63% 21% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12610 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 CoA transferase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2471	1547	449	466	9			
1	B	353	Total	C	N	O	S	0	0	0
			2562	1615	459	478	10			
1	C	354	Total	C	N	O	S	0	0	0
			2500	1572	445	473	10			
1	D	352	Total	C	N	O	S	0	0	0
			2524	1587	448	479	10			
1	E	344	Total	C	N	O	S	0	0	0
			2410	1517	427	456	10			

- Molecule 2 is water.

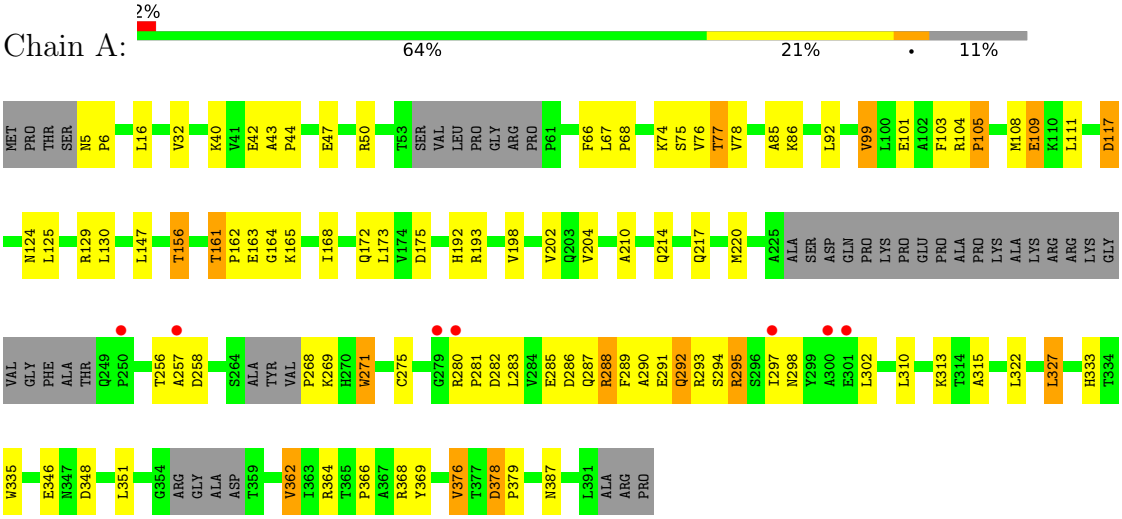
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total	O	0	0
			39	39		
2	B	32	Total	O	0	0
			32	32		
2	C	30	Total	O	0	0
			30	30		
2	D	23	Total	O	0	0
			23	23		
2	E	19	Total	O	0	0
			19	19		

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.

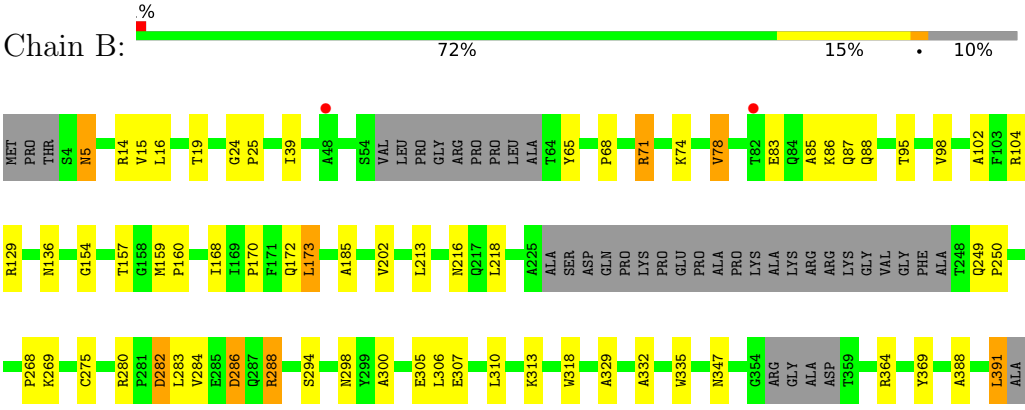
• Molecule 1: CoA transferase III

Chain A:



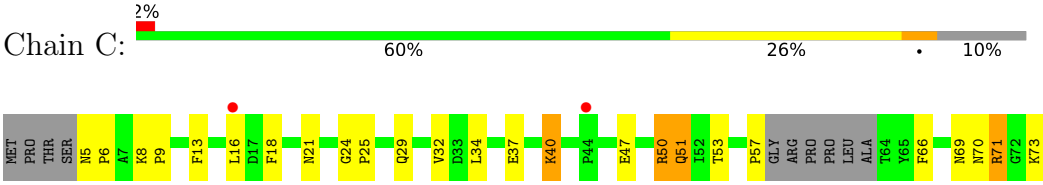
• Molecule 1: CoA transferase III

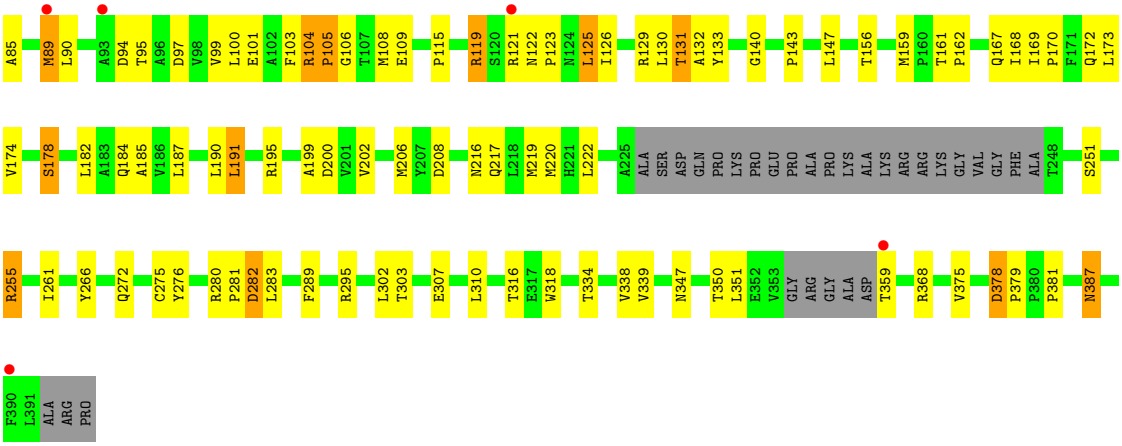
Chain B:



• Molecule 1: CoA transferase III

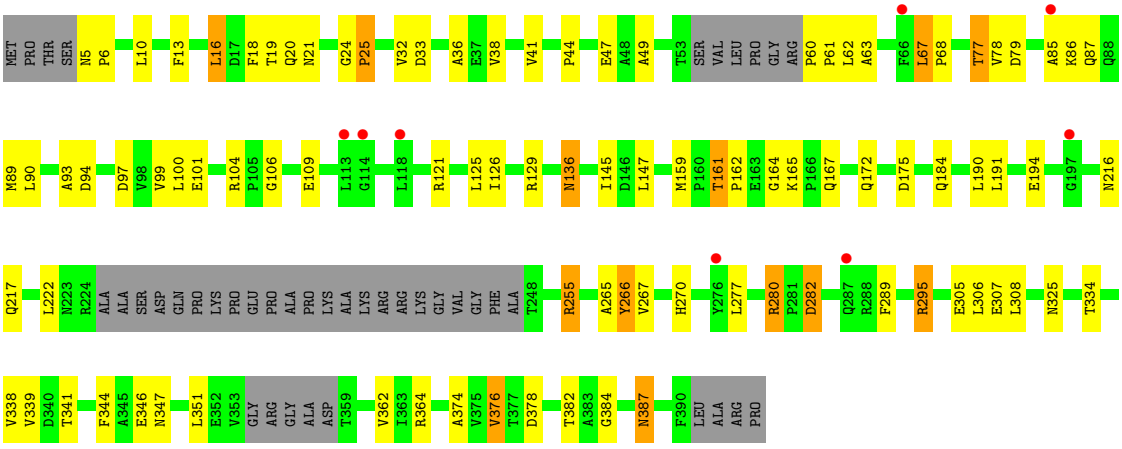
Chain C:





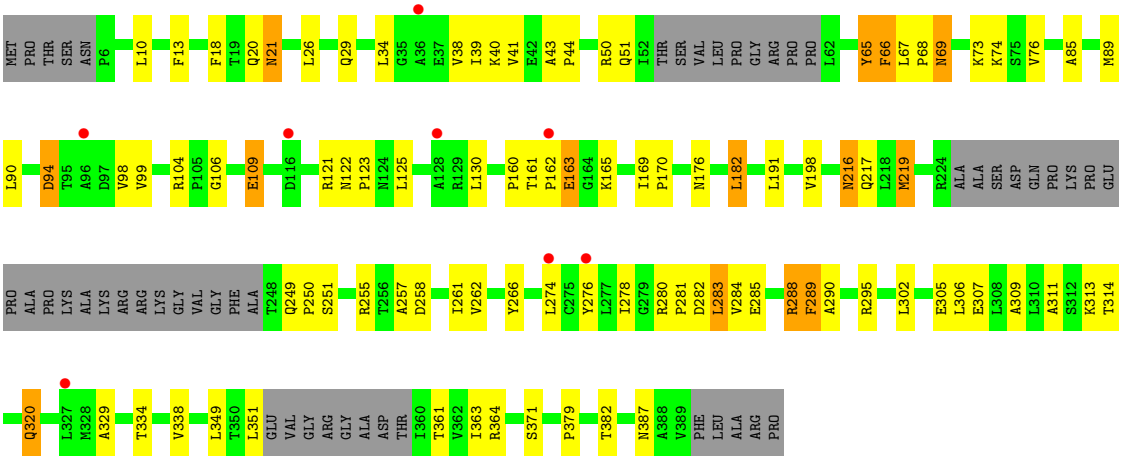
• Molecule 1: CoA transferase III

Chain D:



• Molecule 1: CoA transferase III

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	542.40Å 71.00Å 49.55Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	43.59 – 2.79 43.59 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.59-2.79) 96.9 (43.59-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.231 , 0.286 0.231 , 0.286	Depositor DCC
R_{free} test set	2260 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12610	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 4.57% 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	0.69	0/2515	0.75	0/3439
1	B	0.71	0/2611	0.78	0/3571
1	C	0.66	0/2547	0.75	1/3486 (0.0%)
1	D	0.68	0/2572	0.77	4/3517 (0.1%)
1	E	0.72	0/2457	0.79	1/3366 (0.0%)
All	All	0.69	0/12702	0.77	6/17379 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	PRO	N-CA-CB	6.75	111.39	103.30
1	D	61	PRO	N-CA-CB	5.88	110.36	103.30
1	D	60	PRO	N-CA-CB	5.75	110.19	103.30
1	D	60	PRO	N-CA-C	-5.57	97.63	112.10
1	E	123	PRO	N-CA-CB	5.48	109.88	103.30
1	D	44	PRO	N-CA-CB	5.28	109.64	103.30

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	2471	0	2276	90	0
1	B	2562	0	2436	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2500	0	2296	112	0
1	D	2524	0	2340	89	0
1	E	2410	0	2184	80	0
2	A	39	0	0	0	0
2	B	32	0	0	0	0
2	C	30	0	0	2	0
2	D	23	0	0	1	0
2	E	19	0	0	0	0
All	All	12610	0	11532	399	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 (399) 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:256:THR:HA	1:A:310:LEU:O	1.41	1.20
1:D:77:THR:H	1:D:387:ASN:ND2	1.42	1.16
1:D:77:THR:N	1:D:387:ASN:HD21	1.45	1.14
1:C:40:LYS:NZ	1:C:70:ASN:HD21	1.60	0.98
1:A:258:ASP:O	1:A:315:ALA:HB2	1.66	0.95
1:E:161:THR:HB	1:E:162:PRO:HD2	1.50	0.93
1:A:257:ALA:HB3	1:A:313:LYS:O	1.67	0.93
1:D:77:THR:N	1:D:387:ASN:ND2	2.11	0.92
1:C:50:ARG:NH2	1:C:381:PRO:O	2.05	0.89
1:D:77:THR:H	1:D:387:ASN:HD21	0.93	0.89
1:A:256:THR:CA	1:A:310:LEU:O	2.22	0.87
1:E:10:LEU:O	1:E:13:PHE:HD2	1.57	0.87
1:C:40:LYS:CE	1:C:70:ASN:ND2	2.39	0.86
1:C:115:PRO:O	1:C:119:ARG:HB2	1.74	0.85
1:E:278:ILE:HD12	1:E:309:ALA:CB	2.06	0.85
1:C:77:THR:H	1:C:387:ASN:ND2	1.75	0.83
1:C:40:LYS:HZ1	1:C:70:ASN:HD21	1.27	0.82
1:C:122:ASN:OD1	1:C:123:PRO:HD2	1.79	0.82
1:E:351:LEU:C	1:E:351:LEU:HD12	2.01	0.81
1:A:103:PHE:CE2	1:A:108:MET:HE3	2.15	0.81
1:A:217:GLN:NE2	1:B:172:GLN:HE22	1.79	0.81
1:A:257:ALA:CB	1:A:313:LYS:O	2.30	0.80
1:D:94:ASP:OD2	1:D:121:ARG:HD3	1.83	0.79
1:D:161:THR:HG22	1:D:164:GLY:H	1.47	0.79
1:E:351:LEU:HD23	1:E:364:ARG:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:HB2	1:A:298:ASN:HD22	1.46	0.79
1:A:67:LEU:N	1:A:68:PRO:HD2	1.98	0.78
1:A:217:GLN:HE21	1:B:172:GLN:HE22	1.28	0.78
1:D:384:GLY:HA2	1:D:387:ASN:HD22	1.48	0.77
1:A:288:ARG:HB3	1:A:298:ASN:ND2	1.99	0.77
1:A:103:PHE:HE2	1:A:108:MET:HE3	1.47	0.77
1:A:288:ARG:CB	1:A:298:ASN:ND2	2.47	0.77
1:D:280:ARG:HG2	1:D:280:ARG:HH11	1.48	0.76
1:C:77:THR:H	1:C:387:ASN:HD21	1.34	0.75
1:E:255:ARG:HB2	1:E:307:GLU:OE2	1.86	0.75
1:C:40:LYS:NZ	1:C:70:ASN:ND2	2.35	0.75
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.68	0.74
1:D:270:HIS:ND1	2:D:401:HOH:O	2.22	0.73
1:A:109:GLU:OE1	1:A:129:ARG:NH2	2.21	0.73
1:C:161:THR:CG2	2:C:424:HOH:O	2.38	0.72
1:B:19:THR:HG22	1:B:102:ALA:CB	2.21	0.71
1:A:156:THR:HG21	1:B:332:ALA:HB1	1.71	0.71
1:D:77:THR:CA	1:D:387:ASN:HD21	2.04	0.71
1:D:68:PRO:HD3	1:D:362:VAL:HG11	1.74	0.70
1:D:19:THR:HB	1:D:25:PRO:HD3	1.74	0.70
1:E:161:THR:HB	1:E:162:PRO:CD	2.21	0.70
1:A:68:PRO:HA	1:A:362:VAL:HG11	1.74	0.69
1:D:18:PHE:CE1	1:D:41:VAL:HG11	2.28	0.69
1:C:40:LYS:HE2	1:C:70:ASN:ND2	2.08	0.69
1:D:282:ASP:OD1	1:D:282:ASP:N	2.22	0.69
1:C:222:LEU:HD23	1:D:339:VAL:HG11	1.76	0.68
1:C:104:ARG:HH11	1:C:143:PRO:HD3	1.57	0.68
1:A:292:GLN:O	1:A:295:ARG:HD2	1.93	0.68
1:D:255:ARG:HG3	1:D:307:GLU:OE2	1.93	0.68
1:C:368:ARG:HH12	1:D:136:ASN:HD21	1.40	0.67
1:C:289:PHE:CE1	1:C:302:LEU:HB2	2.29	0.67
1:B:255:ARG:HB2	1:B:307:GLU:OE2	1.94	0.67
1:C:13:PHE:HD1	1:C:97:ASP:OD2	1.77	0.67
1:D:5:ASN:CB	1:D:6:PRO:HD3	2.25	0.66
1:A:271:TRP:HE3	1:A:271:TRP:O	1.79	0.66
1:C:104:ARG:NH1	1:C:143:PRO:HD3	2.10	0.66
1:C:71:ARG:NH1	1:C:351:LEU:HD21	2.10	0.66
1:E:295:ARG:HG2	1:E:302:LEU:HD22	1.76	0.66
1:E:282:ASP:OD1	1:E:282:ASP:N	2.25	0.65
1:E:94:ASP:O	1:E:122:ASN:ND2	2.29	0.65
1:C:109:GLU:OE2	1:C:129:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:CG1	1:A:125:LEU:HD11	2.27	0.65
1:C:282:ASP:OD1	1:C:282:ASP:N	2.23	0.65
1:C:351:LEU:HD12	1:C:351:LEU:O	1.97	0.64
1:B:14:ARG:HH11	1:B:95:THR:CG2	2.09	0.64
1:C:32:VAL:HG21	1:C:73:LYS:HG2	1.79	0.64
1:C:351:LEU:HD12	1:C:351:LEU:C	2.18	0.64
1:E:106:GLY:HA2	1:E:109:GLU:OE2	1.97	0.64
1:D:280:ARG:HG2	1:D:280:ARG:NH1	2.14	0.63
1:B:14:ARG:NH1	1:B:95:THR:HG21	2.13	0.63
1:E:290:ALA:O	1:E:295:ARG:NH2	2.28	0.63
1:A:288:ARG:CB	1:A:298:ASN:HD22	2.08	0.63
1:B:282:ASP:OD1	1:B:282:ASP:N	2.23	0.63
1:C:40:LYS:CE	1:C:70:ASN:HD21	2.08	0.63
1:D:161:THR:HG23	1:D:162:PRO:HD2	1.80	0.63
1:E:10:LEU:C	1:E:13:PHE:HD2	2.02	0.63
1:A:333:HIS:O	1:B:154:GLY:HA2	1.98	0.63
1:C:40:LYS:CD	1:C:70:ASN:HD22	2.12	0.63
1:C:170:PRO:CD	1:D:159:MET:HE2	2.29	0.63
1:B:19:THR:HG22	1:B:102:ALA:HB2	1.81	0.62
1:D:384:GLY:CA	1:D:387:ASN:HD22	2.12	0.62
1:A:103:PHE:CE2	1:A:108:MET:CE	2.82	0.62
1:E:67:LEU:N	1:E:68:PRO:CD	2.62	0.62
1:A:258:ASP:O	1:A:315:ALA:CB	2.45	0.61
1:B:14:ARG:HH11	1:B:95:THR:HG21	1.64	0.61
1:E:106:GLY:HA2	1:E:109:GLU:CD	2.19	0.61
1:A:288:ARG:HB3	1:A:298:ASN:HD21	1.65	0.61
1:D:109:GLU:OE2	1:D:129:ARG:NH2	2.33	0.61
1:C:100:LEU:HD12	1:C:100:LEU:N	2.16	0.61
1:A:103:PHE:CD2	1:A:108:MET:HE2	2.36	0.61
1:A:76:VAL:HA	1:A:387:ASN:OD1	2.01	0.60
1:B:294:SER:O	1:B:298:ASN:HB2	2.02	0.60
1:A:67:LEU:N	1:A:68:PRO:CD	2.64	0.60
1:C:302:LEU:HD12	1:C:302:LEU:O	2.00	0.60
1:C:161:THR:CG2	1:C:162:PRO:HD2	2.32	0.60
1:D:280:ARG:HH22	1:D:305:GLU:CD	2.03	0.60
1:A:322:LEU:O	1:A:327:LEU:HB2	2.01	0.59
1:A:346:GLU:HG2	1:B:136:ASN:O	2.01	0.59
1:C:172:GLN:HE22	1:D:217:GLN:NE2	1.99	0.59
1:D:136:ASN:OD1	1:D:136:ASN:N	2.25	0.59
1:A:103:PHE:CD2	1:A:108:MET:CE	2.85	0.59
1:A:161:THR:HG22	1:A:164:GLY:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:MET:HE2	1:D:68:PRO:CG	2.31	0.59
1:C:5:ASN:N	1:C:6:PRO:HD2	2.17	0.59
1:C:303:THR:O	1:C:307:GLU:HG3	2.03	0.59
1:E:43:ALA:HB1	1:E:44:PRO:HD2	1.85	0.59
1:C:174:VAL:O	1:C:178:SER:OG	2.21	0.58
1:C:40:LYS:HE3	1:C:47:GLU:OE2	2.04	0.58
1:D:62:LEU:O	1:D:63:ALA:HB3	2.03	0.58
1:A:161:THR:HG23	1:A:162:PRO:HD2	1.85	0.58
1:E:283:LEU:O	1:E:284:VAL:C	2.36	0.58
1:B:255:ARG:N	1:B:307:GLU:OE2	2.26	0.58
1:E:278:ILE:HD12	1:E:309:ALA:HB1	1.81	0.58
1:D:5:ASN:CB	1:D:6:PRO:CD	2.82	0.57
1:E:90:LEU:CB	1:E:121:ARG:NH1	2.67	0.57
1:B:168:ILE:O	1:B:170:PRO:HD3	2.05	0.57
1:E:305:GLU:OE1	1:E:305:GLU:HA	2.05	0.57
1:C:131:THR:HB	1:C:133:TYR:O	2.04	0.57
1:D:33:ASP:HB3	1:D:374:ALA:HB1	1.86	0.57
1:B:282:ASP:O	1:B:286:ASP:HB3	2.05	0.56
1:B:268:PRO:HG2	1:B:269:LYS:H	1.70	0.56
1:D:376:VAL:HG12	1:D:376:VAL:O	2.05	0.56
1:E:280:ARG:HB3	1:E:283:LEU:HD22	1.88	0.56
1:B:109:GLU:OE1	1:B:109:GLU:N	2.36	0.56
1:E:255:ARG:CB	1:E:307:GLU:OE2	2.54	0.56
1:A:282:ASP:N	1:A:282:ASP:OD1	2.37	0.56
1:A:103:PHE:HD2	1:A:108:MET:HE2	1.70	0.56
1:C:16:LEU:HB3	1:C:18:PHE:HE1	1.70	0.56
1:A:368:ARG:NH2	1:B:136:ASN:OD1	2.39	0.56
1:C:40:LYS:CD	1:C:70:ASN:ND2	2.69	0.56
1:C:101:GLU:HG3	1:C:108:MET:HG3	1.88	0.56
1:A:282:ASP:HA	1:A:285:GLU:CB	2.36	0.56
1:C:101:GLU:OE2	1:C:129:ARG:CD	2.55	0.55
1:B:15:VAL:HG13	1:B:98:VAL:HB	1.88	0.55
1:C:170:PRO:HD3	1:D:159:MET:CE	2.36	0.55
1:E:288:ARG:HH11	1:E:288:ARG:CG	2.18	0.55
1:A:378:ASP:OD1	1:A:378:ASP:N	2.37	0.55
1:C:130:LEU:HD13	1:C:182:LEU:HD22	1.88	0.55
1:C:347:ASN:O	1:C:368:ARG:NH2	2.39	0.55
1:C:208:ASP:OD2	1:D:364:ARG:NH2	2.40	0.54
1:D:351:LEU:C	1:D:351:LEU:HD12	2.26	0.54
1:D:18:PHE:HB2	1:D:100:LEU:O	2.06	0.54
1:A:47:GLU:HG3	1:A:47:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLU:HG3	1:A:108:MET:HG3	1.88	0.54
1:B:39:ILE:HG23	1:B:74:LYS:HB2	1.89	0.54
1:C:101:GLU:OE2	1:C:129:ARG:HD2	2.07	0.54
1:A:117:ASP:N	1:A:117:ASP:OD1	2.41	0.53
1:E:10:LEU:O	1:E:13:PHE:CD2	2.49	0.53
1:B:170:PRO:HB2	1:B:335:TRP:HH2	1.73	0.53
1:A:147:LEU:HD21	1:A:168:ILE:HD13	1.90	0.53
1:E:161:THR:CB	1:E:162:PRO:HD2	2.31	0.53
1:C:170:PRO:HD2	1:D:159:MET:HE2	1.91	0.53
1:C:217:GLN:NE2	1:D:172:GLN:OE1	2.42	0.53
1:E:76:VAL:HA	1:E:387:ASN:OD1	2.08	0.53
1:B:388:ALA:H	1:B:391:LEU:HB2	1.72	0.53
1:C:97:ASP:O	1:C:125:LEU:HA	2.09	0.53
1:A:86:LYS:HD2	1:A:111:LEU:O	2.09	0.53
1:C:351:LEU:HD22	1:C:375:VAL:HG13	1.90	0.53
1:A:78:VAL:HG13	1:A:85:ALA:HB1	1.91	0.52
1:A:42:GLU:OE1	1:A:75:SER:CB	2.57	0.52
1:A:271:TRP:HE3	1:A:271:TRP:C	2.12	0.52
1:E:67:LEU:N	1:E:68:PRO:HD2	2.25	0.52
1:A:286:ASP:CB	1:A:288:ARG:HD2	2.40	0.52
1:B:347:ASN:O	1:B:364:ARG:NH2	2.36	0.52
1:C:9:PRO:HD2	1:C:34:LEU:O	2.09	0.52
1:C:368:ARG:HH12	1:D:136:ASN:ND2	2.07	0.52
1:B:85:ALA:O	1:B:86:LYS:C	2.48	0.52
1:D:32:VAL:HG23	1:D:38:VAL:HG21	1.91	0.52
1:D:77:THR:CB	1:D:387:ASN:HD21	2.22	0.52
1:B:313:LYS:HD2	1:B:318:TRP:CZ2	2.45	0.51
1:A:99:VAL:HG12	1:A:125:LEU:HD11	1.91	0.51
1:A:288:ARG:HB2	1:A:298:ASN:ND2	2.11	0.51
1:B:78:VAL:HG22	1:B:85:ALA:CB	2.40	0.51
1:C:29:GLN:HB2	1:C:69:ASN:O	2.11	0.51
1:D:351:LEU:HD12	1:D:351:LEU:O	2.10	0.51
1:E:283:LEU:CD1	1:E:283:LEU:N	2.73	0.51
1:C:50:ARG:HB2	1:C:51:GLN:NE2	2.27	0.50
1:E:99:VAL:HG23	1:E:125:LEU:HD11	1.92	0.50
1:B:109:GLU:CD	1:B:129:ARG:HH22	2.15	0.50
1:A:124:ASN:O	1:A:193:ARG:NH1	2.39	0.50
1:C:13:PHE:CD1	1:C:97:ASP:OD2	2.63	0.50
1:A:130:LEU:HD12	1:A:204:VAL:HG12	1.93	0.50
1:B:256:THR:HG22	1:B:310:LEU:HB3	1.94	0.49
1:C:170:PRO:CD	1:D:159:MET:CE	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:ARG:HG3	1:E:289:PHE:CZ	2.48	0.49
1:C:219:MET:HE2	1:D:68:PRO:HG2	1.93	0.49
1:D:32:VAL:HG23	1:D:38:VAL:CG2	2.43	0.49
1:D:266:TYR:O	1:D:295:ARG:NH2	2.46	0.49
1:A:378:ASP:HB3	1:A:379:PRO:HD2	1.95	0.49
1:E:67:LEU:CB	1:E:68:PRO:HD3	2.42	0.49
1:D:126:ILE:HD12	1:D:190:LEU:HD23	1.94	0.49
1:D:161:THR:HG21	1:D:165:LYS:HG2	1.94	0.49
1:E:10:LEU:HD12	1:E:34:LEU:HB2	1.95	0.49
1:D:13:PHE:HD1	1:D:97:ASP:OD2	1.96	0.48
1:D:99:VAL:HG23	1:D:125:LEU:HD11	1.95	0.48
1:A:44:PRO:HA	1:A:77:THR:HG23	1.94	0.48
1:E:66:PHE:CD1	1:E:66:PHE:C	2.86	0.48
1:E:257:ALA:HB2	1:E:311:ALA:O	2.13	0.48
1:C:161:THR:HG22	1:C:162:PRO:HD2	1.94	0.48
1:D:161:THR:HG22	1:D:164:GLY:N	2.21	0.48
1:E:334:THR:O	1:E:338:VAL:HG23	2.13	0.48
1:C:47:GLU:HB3	1:C:50:ARG:HG3	1.96	0.48
1:D:20:GLN:O	1:D:21:ASN:HB2	2.14	0.48
1:E:289:PHE:HB3	1:E:295:ARG:HG3	1.94	0.48
1:C:161:THR:HG23	1:C:162:PRO:HD2	1.96	0.48
1:A:104:ARG:HD2	1:A:105:PRO:HD2	1.96	0.48
1:D:255:ARG:CG	1:D:307:GLU:OE2	2.60	0.48
1:B:19:THR:HG22	1:B:102:ALA:HB3	1.96	0.48
1:E:98:VAL:HG12	1:E:99:VAL:N	2.29	0.48
1:A:268:PRO:N	1:A:292:GLN:HE22	2.12	0.48
1:C:276:TYR:HE1	1:C:281:PRO:HB3	1.79	0.48
1:B:268:PRO:CG	1:B:269:LYS:H	2.26	0.47
1:E:276:TYR:HE1	1:E:281:PRO:HB3	1.79	0.47
1:E:387:ASN:OD1	1:E:387:ASN:N	2.46	0.47
1:A:173:LEU:HD12	1:B:173:LEU:HD13	1.94	0.47
1:C:156:THR:HG22	1:C:167:GLN:O	2.14	0.47
1:C:222:LEU:HD23	1:D:339:VAL:CG1	2.42	0.47
1:E:288:ARG:CG	1:E:288:ARG:NH1	2.77	0.47
1:B:154:GLY:O	1:B:157:THR:OG1	2.29	0.47
1:C:219:MET:HE2	1:D:68:PRO:HG3	1.96	0.47
1:E:69:ASN:O	1:E:73:LYS:NZ	2.48	0.47
1:A:192:HIS:CE1	1:A:198:VAL:HG11	2.50	0.47
1:B:88:GLN:OE1	1:B:391:LEU:HD13	2.15	0.47
1:D:341:THR:OG1	1:D:344:PHE:HB2	2.15	0.47
1:D:305:GLU:HA	1:D:305:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLY:N	1:C:25:PRO:CD	2.78	0.47
1:D:277:LEU:HD11	1:D:325:ASN:CB	2.45	0.47
1:A:66:PHE:CD1	1:A:66:PHE:C	2.88	0.47
1:B:313:LYS:HD2	1:B:318:TRP:CH2	2.50	0.47
1:B:313:LYS:HB2	1:B:318:TRP:CE2	2.50	0.47
1:C:109:GLU:CD	1:C:129:ARG:HH22	2.18	0.46
1:C:316:THR:HG23	2:C:417:HOH:O	2.14	0.46
1:B:24:GLY:N	1:B:25:PRO:CD	2.78	0.46
1:B:268:PRO:HG2	1:B:269:LYS:N	2.30	0.46
1:C:251:SER:OG	1:D:147:LEU:HD13	2.15	0.46
1:D:16:LEU:HD12	1:D:18:PHE:CE2	2.50	0.46
1:D:87:GLN:OE1	1:D:87:GLN:HA	2.15	0.46
1:E:90:LEU:C	1:E:121:ARG:HH12	2.18	0.46
1:C:208:ASP:OD1	1:D:347:ASN:ND2	2.45	0.46
1:C:94:ASP:OD2	1:C:121:ARG:NH1	2.49	0.46
1:C:289:PHE:HA	1:C:295:ARG:HG3	1.97	0.46
1:A:16:LEU:HD11	1:A:92:LEU:HG	1.97	0.46
1:B:83:GLU:O	1:B:87:GLN:HG2	2.15	0.46
1:A:50:ARG:CZ	1:A:66:PHE:CZ	2.98	0.46
1:C:334:THR:O	1:C:338:VAL:HG23	2.15	0.46
1:B:78:VAL:HG22	1:B:85:ALA:HB1	1.98	0.46
1:E:349:LEU:O	1:E:364:ARG:HG2	2.14	0.46
1:A:192:HIS:NE2	1:A:198:VAL:HG11	2.31	0.46
1:E:219:MET:O	1:E:219:MET:HG3	2.14	0.46
1:E:94:ASP:OD1	1:E:121:ARG:CZ	2.64	0.45
1:E:302:LEU:HD12	1:E:302:LEU:O	2.16	0.45
1:A:161:THR:HG21	1:A:165:LYS:HB3	1.97	0.45
1:C:13:PHE:HA	1:C:97:ASP:OD2	2.16	0.45
1:E:40:LYS:O	1:E:76:VAL:HG22	2.16	0.45
1:B:275:CYS:HB2	1:B:284:VAL:HG22	1.97	0.45
1:D:384:GLY:O	1:D:387:ASN:HB2	2.16	0.45
1:E:283:LEU:N	1:E:283:LEU:HD13	2.32	0.45
1:C:276:TYR:CE1	1:C:281:PRO:HB3	2.51	0.45
1:A:289:PHE:O	1:A:294:SER:HB2	2.16	0.45
1:D:277:LEU:HD21	1:D:325:ASN:ND2	2.31	0.45
1:E:278:ILE:HD12	1:E:309:ALA:HB3	1.93	0.45
1:A:298:ASN:O	1:A:302:LEU:N	2.42	0.45
1:C:101:GLU:OE2	1:C:129:ARG:HD3	2.17	0.45
1:C:169:ILE:HA	1:D:159:MET:HE1	1.99	0.45
1:E:85:ALA:O	1:E:89:MET:HG2	2.17	0.45
1:A:103:PHE:HD2	1:A:108:MET:CE	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:MET:O	1:D:93:ALA:N	2.45	0.45
1:E:249:GLN:HB3	1:E:250:PRO:HA	1.98	0.45
1:B:68:PRO:O	1:B:71:ARG:NH1	2.50	0.45
1:B:268:PRO:CG	1:B:269:LYS:N	2.80	0.45
1:D:19:THR:HB	1:D:24:GLY:HA3	1.99	0.44
1:C:351:LEU:HD22	1:C:375:VAL:CG1	2.48	0.44
1:D:10:LEU:HB3	1:D:36:ALA:HB2	2.00	0.44
1:B:262:VAL:O	1:B:329:ALA:HA	2.17	0.44
1:D:277:LEU:HD11	1:D:325:ASN:CG	2.37	0.44
1:E:10:LEU:C	1:E:13:PHE:CD2	2.88	0.44
1:D:334:THR:O	1:D:338:VAL:HG23	2.17	0.44
1:E:191:LEU:HD23	1:E:191:LEU:HA	1.54	0.44
1:A:210:ALA:O	1:A:214:GLN:HG3	2.17	0.44
1:C:51:GLN:NE2	1:C:51:GLN:N	2.66	0.44
1:D:47:GLU:HG2	1:D:49:ALA:H	1.82	0.44
1:D:79:ASP:O	1:D:85:ALA:HB2	2.17	0.44
1:C:99:VAL:C	1:C:100:LEU:HD12	2.38	0.44
1:C:280:ARG:CB	1:C:283:LEU:HD12	2.48	0.44
1:E:258:ASP:HB3	1:E:314:THR:HG22	1.99	0.44
1:A:287:GLN:O	1:A:290:ALA:CB	2.66	0.44
1:B:5:ASN:O	1:B:5:ASN:OD1	2.36	0.44
1:B:14:ARG:NH1	1:B:95:THR:CG2	2.77	0.44
1:D:19:THR:CB	1:D:25:PRO:HD3	2.45	0.44
1:D:308:LEU:HD23	1:D:308:LEU:HA	1.81	0.44
1:E:169:ILE:HA	1:E:170:PRO:HD3	1.78	0.44
1:A:275:CYS:O	1:A:280:ARG:O	2.35	0.44
1:C:159:MET:HE2	1:D:167:GLN:CG	2.48	0.43
1:C:310:LEU:HD23	1:C:318:TRP:CE2	2.52	0.43
1:D:161:THR:HG23	1:D:162:PRO:CD	2.45	0.43
1:A:68:PRO:HA	1:A:362:VAL:CG1	2.45	0.43
1:A:173:LEU:H	1:A:173:LEU:HD23	1.83	0.43
1:B:159:MET:HA	1:B:160:PRO:HD3	1.84	0.43
1:C:104:ARG:HD2	1:C:105:PRO:HD2	1.99	0.43
1:C:275:CYS:HB3	1:C:280:ARG:O	2.17	0.43
1:D:79:ASP:O	1:D:85:ALA:CB	2.66	0.43
1:A:288:ARG:O	1:A:294:SER:HB3	2.17	0.43
1:E:219:MET:HE3	1:E:219:MET:HB2	1.84	0.43
1:A:32:VAL:HG12	1:A:376:VAL:HG11	2.00	0.43
1:E:74:LYS:N	1:E:74:LYS:CD	2.81	0.43
1:A:280:ARG:HA	1:A:281:PRO:HD3	1.83	0.43
1:B:14:ARG:HH11	1:B:95:THR:HG23	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:LEU:CB	1:E:121:ARG:HH11	2.31	0.43
1:C:50:ARG:HH21	1:C:66:PHE:HZ	1.66	0.43
1:C:21:ASN:O	1:C:25:PRO:HG2	2.19	0.43
1:E:20:GLN:O	1:E:21:ASN:HB2	2.18	0.43
1:E:274:LEU:O	1:E:274:LEU:HG	2.19	0.43
1:E:283:LEU:HD13	1:E:283:LEU:H	1.83	0.43
1:A:40:LYS:HG3	1:A:74:LYS:O	2.18	0.43
1:C:378:ASP:OD1	1:C:378:ASP:N	2.50	0.43
1:D:67:LEU:CB	1:D:68:PRO:HD2	2.49	0.43
1:E:262:VAL:O	1:E:329:ALA:HA	2.18	0.43
1:C:101:GLU:HG3	1:C:108:MET:CG	2.49	0.43
1:E:98:VAL:CG1	1:E:99:VAL:N	2.81	0.43
1:C:50:ARG:HB2	1:C:51:GLN:HE22	1.84	0.43
1:A:217:GLN:HE21	1:B:172:GLN:NE2	2.07	0.42
1:C:125:LEU:O	1:C:199:ALA:HB1	2.19	0.42
1:E:283:LEU:O	1:E:285:GLU:N	2.52	0.42
1:E:29:GLN:HB2	1:E:69:ASN:O	2.19	0.42
1:A:66:PHE:C	1:A:68:PRO:HD2	2.39	0.42
1:A:202:VAL:HG22	1:B:369:TYR:CD2	2.54	0.42
1:B:280:ARG:NH2	1:B:305:GLU:OE1	2.52	0.42
1:A:99:VAL:HG13	1:A:125:LEU:HD11	1.97	0.42
1:A:172:GLN:HB3	1:A:175:ASP:HB2	2.01	0.42
1:A:364:ARG:NH1	1:A:366:PRO:HA	2.35	0.42
1:B:249:GLN:HA	1:B:250:PRO:HA	1.67	0.42
1:E:216:ASN:ND2	1:E:217:GLN:HE21	2.17	0.42
1:A:287:GLN:O	1:A:290:ALA:HB2	2.19	0.42
1:C:71:ARG:H	1:C:71:ARG:HG2	1.57	0.42
1:C:85:ALA:O	1:C:89:MET:N	2.47	0.42
1:E:38:VAL:HG12	1:E:39:ILE:N	2.34	0.42
1:E:66:PHE:O	1:E:66:PHE:CG	2.72	0.42
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.67	0.42
1:E:161:THR:CB	1:E:162:PRO:CD	2.86	0.42
1:A:5:ASN:N	1:A:6:PRO:HD3	2.34	0.42
1:B:283:LEU:N	1:B:283:LEU:CD1	2.82	0.42
1:D:106:GLY:HA2	1:D:109:GLU:OE1	2.20	0.42
1:C:5:ASN:N	1:C:6:PRO:CD	2.81	0.42
1:C:100:LEU:N	1:C:100:LEU:CD1	2.83	0.42
1:C:8:LYS:HB3	1:C:34:LEU:O	2.20	0.42
1:C:71:ARG:NH1	1:C:351:LEU:CD2	2.81	0.42
1:C:185:ALA:HB1	1:C:202:VAL:HG11	2.02	0.41
1:E:65:TYR:CD2	1:E:65:TYR:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:H	1:A:288:ARG:HG3	1.50	0.41
1:C:126:ILE:CD1	1:C:190:LEU:HD23	2.50	0.41
1:E:130:LEU:HD13	1:E:182:LEU:HD22	2.02	0.41
1:A:271:TRP:CZ2	1:A:289:PHE:CB	3.03	0.41
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.85	0.41
1:C:132:ALA:HA	1:C:206:MET:CE	2.51	0.41
1:C:216:ASN:O	1:C:220:MET:HG2	2.20	0.41
1:E:26:LEU:HD22	1:E:176:ASN:ND2	2.35	0.41
1:A:271:TRP:C	1:A:271:TRP:CE3	2.94	0.41
1:C:140:GLY:N	1:D:346:GLU:OE2	2.48	0.41
1:D:191:LEU:HD23	1:D:191:LEU:HA	1.74	0.41
1:D:306:LEU:HD23	1:D:306:LEU:HA	1.81	0.41
1:E:50:ARG:HH22	1:E:382:THR:HA	1.85	0.41
1:C:101:GLU:HG2	1:C:103:PHE:H	1.84	0.41
1:E:41:VAL:HA	1:E:76:VAL:HG23	2.02	0.41
1:C:50:ARG:HG2	1:C:66:PHE:CD2	2.55	0.41
1:A:335:TRP:HB3	1:B:218:LEU:HD23	2.02	0.41
1:B:185:ALA:HB1	1:B:202:VAL:CG1	2.51	0.41
1:B:275:CYS:HB3	1:B:280:ARG:O	2.20	0.41
1:C:40:LYS:CE	1:C:47:GLU:OE2	2.69	0.41
1:C:255:ARG:HB2	1:C:307:GLU:OE2	2.20	0.41
1:D:67:LEU:CB	1:D:68:PRO:CD	2.98	0.41
1:D:265:ALA:O	1:D:267:VAL:N	2.48	0.41
1:E:320:GLN:HE21	1:E:320:GLN:HB2	1.58	0.41
1:C:104:ARG:O	1:C:106:GLY:N	2.54	0.41
1:C:184:GLN:HB2	1:D:184:GLN:HB2	2.02	0.41
1:E:18:PHE:CD1	1:E:18:PHE:N	2.89	0.41
1:E:163:GLU:H	1:E:163:GLU:HG2	1.70	0.41
1:A:369:TYR:CD1	1:A:369:TYR:N	2.89	0.41
1:B:173:LEU:HD11	1:B:213:LEU:HD13	2.02	0.41
1:B:185:ALA:HB1	1:B:202:VAL:HG11	2.03	0.41
1:B:286:ASP:OD2	1:B:288:ARG:NH1	2.54	0.41
1:C:115:PRO:HG3	1:C:129:ARG:NH2	2.36	0.41
1:A:40:LYS:HE2	1:A:40:LYS:HB3	1.69	0.41
1:A:257:ALA:HB2	1:A:313:LYS:O	2.16	0.41
1:C:147:LEU:HD21	1:C:168:ILE:HD13	2.02	0.40
1:C:191:LEU:HD11	1:D:190:LEU:HB2	2.04	0.40
1:C:378:ASP:HA	1:C:379:PRO:HD2	1.89	0.40
1:A:268:PRO:HB2	1:A:269:LYS:H	1.79	0.40
1:E:65:TYR:O	1:E:65:TYR:CG	2.74	0.40
1:D:289:PHE:O	1:D:295:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:GLN:HB3	1:D:175:ASP:HB2	2.04	0.40
1:E:289:PHE:HB2	1:E:290:ALA:H	1.72	0.40
1:C:339:VAL:HG13	1:D:222:LEU:HD23	2.03	0.40
1:D:89:MET:O	1:D:90:LEU:C	2.60	0.40
1:E:306:LEU:HD23	1:E:306:LEU:HA	1.82	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	340/394 (86%)	324 (95%)	15 (4%)	1 (0%)	41	72
1	B	345/394 (88%)	332 (96%)	11 (3%)	2 (1%)	25	56
1	C	346/394 (88%)	331 (96%)	13 (4%)	2 (1%)	25	56
1	D	344/394 (87%)	323 (94%)	18 (5%)	3 (1%)	17	46
1	E	336/394 (85%)	318 (95%)	12 (4%)	6 (2%)	8	28
All	All	1711/1970 (87%)	1628 (95%)	69 (4%)	14 (1%)	19	49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ILE
1	D	67	LEU
1	D	266	TYR
1	E	198	VAL
1	E	266	TYR
1	B	300	ALA
1	C	125	LEU
1	E	21	ASN
1	B	288	ARG

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Mol	Chain	Res	Type
1	E	160	PRO
1	E	313	LYS
1	C	105	PRO
1	E	379	PRO
1	D	376	VAL

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	222/313 (71%)	200 (90%)	22 (10%)	8 23
1	B	244/313 (78%)	231 (95%)	13 (5%)	22 54
1	C	225/313 (72%)	198 (88%)	27 (12%)	5 15
1	D	233/313 (74%)	214 (92%)	19 (8%)	11 33
1	E	212/313 (68%)	191 (90%)	21 (10%)	8 23
All	All	1136/1565 (73%)	1034 (91%)	102 (9%)	9 28

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	99	VAL
1	A	105	PRO
1	A	109	GLU
1	A	117	ASP
1	A	156	THR
1	A	161	THR
1	A	163	GLU
1	A	220	MET
1	A	271	TRP
1	A	283	LEU
1	A	288	ARG
1	A	291	GLU
1	A	292	GLN

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Mol	Chain	Res	Type
1	A	293	ARG
1	A	295	ARG
1	A	327	LEU
1	A	348	ASP
1	A	351	LEU
1	A	362	VAL
1	A	376	VAL
1	A	378	ASP
1	B	5	ASN
1	B	16	LEU
1	B	65	TYR
1	B	71	ARG
1	B	78	VAL
1	B	104	ARG
1	B	173	LEU
1	B	216	ASN
1	B	255	ARG
1	B	261	ILE
1	B	282	ASP
1	B	286	ASP
1	B	391	LEU
1	C	37	GLU
1	C	40	LYS
1	C	50	ARG
1	C	51	GLN
1	C	53	THR
1	C	71	ARG
1	C	76	VAL
1	C	89	MET
1	C	90	LEU
1	C	95	THR
1	C	104	ARG
1	C	119	ARG
1	C	131	THR
1	C	173	LEU
1	C	178	SER
1	C	191	LEU
1	C	195	ARG
1	C	200	ASP
1	C	255	ARG
1	C	261	ILE
1	C	266	TYR

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Mol	Chain	Res	Type
1	C	272	GLN
1	C	282	ASP
1	C	350	THR
1	C	359	THR
1	C	378	ASP
1	C	387	ASN
1	D	16	LEU
1	D	25	PRO
1	D	77	THR
1	D	78	VAL
1	D	86	LYS
1	D	101	GLU
1	D	104	ARG
1	D	136	ASN
1	D	145	ILE
1	D	161	THR
1	D	194	GLU
1	D	216	ASN
1	D	255	ARG
1	D	280	ARG
1	D	282	ASP
1	D	295	ARG
1	D	378	ASP
1	D	382	THR
1	D	387	ASN
1	E	51	GLN
1	E	65	TYR
1	E	66	PHE
1	E	69	ASN
1	E	94	ASP
1	E	104	ARG
1	E	109	GLU
1	E	163	GLU
1	E	165	LYS
1	E	182	LEU
1	E	216	ASN
1	E	219	MET
1	E	251	SER
1	E	261	ILE
1	E	283	LEU
1	E	288	ARG
1	E	289	PHE

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Mol	Chain	Res	Type
1	E	320	GLN
1	E	361	THR
1	E	363	ILE
1	E	371	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	217	GLN
1	A	298	ASN
1	B	333	HIS
1	C	51	GLN
1	C	70	ASN
1	C	184	GLN
1	C	196	ASN
1	C	387	ASN
1	D	88	GLN
1	D	217	GLN
1	D	325	ASN
1	D	387	ASN
1	E	51	GLN
1	E	176	ASN
1	E	217	GLN
1	E	320	GLN
1	E	323	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	350/394 (88%)	0.04	7 (2%)	65	56	27, 59, 108, 154	0
1	B	353/394 (89%)	-0.09	3 (0%)	86	81	23, 53, 90, 116	0
1	C	354/394 (89%)	0.03	7 (1%)	65	56	32, 68, 104, 124	0
1	D	352/394 (89%)	-0.01	8 (2%)	60	51	30, 67, 98, 114	0
1	E	344/394 (87%)	0.01	8 (2%)	60	51	34, 72, 112, 135	0
All	All	1753/1970 (88%)	-0.01	33 (1%)	66	59	23, 63, 102, 154	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ILE	6.0
1	A	300	ALA	4.3
1	C	89	MET	4.2
1	D	118	LEU	3.6
1	C	359	THR	3.6
1	D	113	LEU	3.4
1	A	257	ALA	2.9
1	C	121	ARG	2.8
1	E	327	LEU	2.7
1	D	276	TYR	2.7
1	B	82	THR	2.7
1	B	111	LEU	2.6
1	C	390	PHE	2.6
1	E	96	ALA	2.6
1	D	85	ALA	2.5
1	D	114	GLY	2.5
1	E	274	LEU	2.5
1	D	197	GLY	2.4
1	E	128	ALA	2.4
1	E	116	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	2.2
1	C	16	LEU	2.2
1	E	36	ALA	2.2
1	D	66	PHE	2.2
1	A	279	GLY	2.1
1	A	301	GLU	2.1
1	A	280	ARG	2.1
1	E	276	TYR	2.1
1	C	93	ALA	2.0
1	A	250	PRO	2.0
1	D	287	GLN	2.0
1	C	44	PRO	2.0
1	E	162	PRO	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.