



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:55 AM EDT

PDB ID : 2GUW / pdb_00002guw
Title : Crystal structure of AMP Nucleosidase from Salmonella typhimurium LT2
Authors : Rao, K.N.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2006-05-01
Resolution : 2.64 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

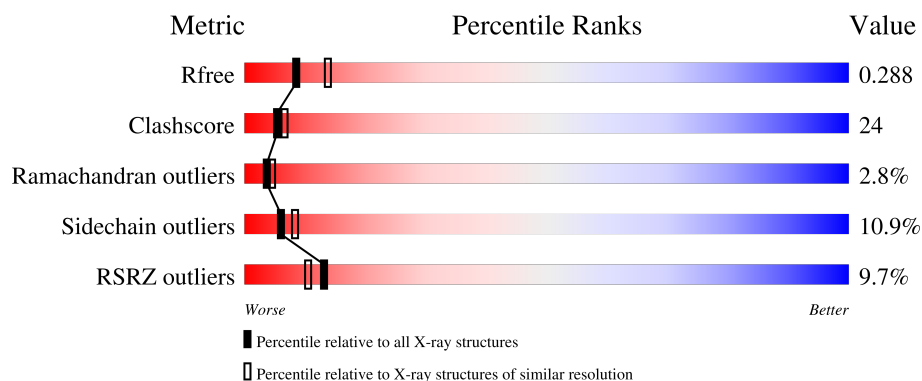
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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 $\leq 5\%$. 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	484	9% 47% 30% 6% 15%
1	B	484	4% 55% 26% 6% 14%
1	C	484	11% 44% 31% 7% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9415 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3182	2018	562	593	9			
1	B	418	Total	C	N	O	S	0	0	0
			3240	2060	561	609	10			
1	C	394	Total	C	N	O	S	0	0	0
			2964	1883	519	554	8			

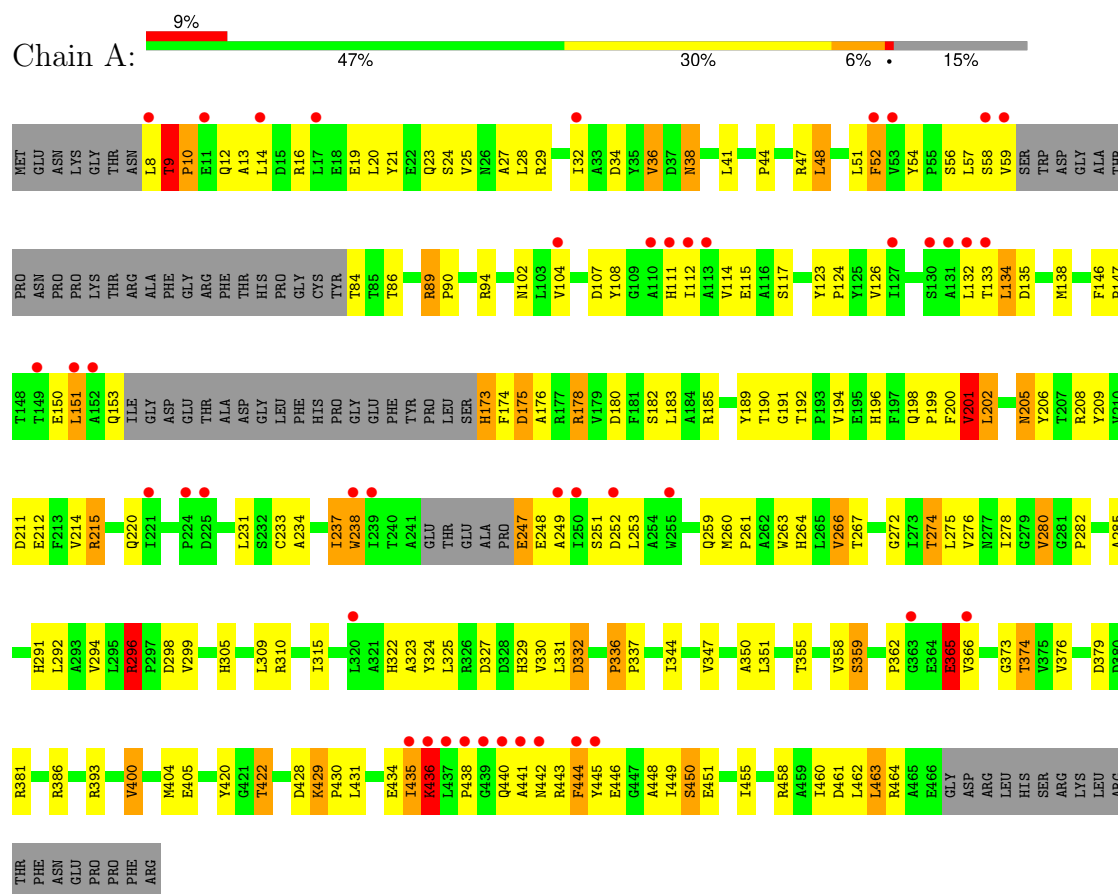
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	13	Total	O	0	0
			13	13		
2	C	3	Total	O	0	0
			3	3		

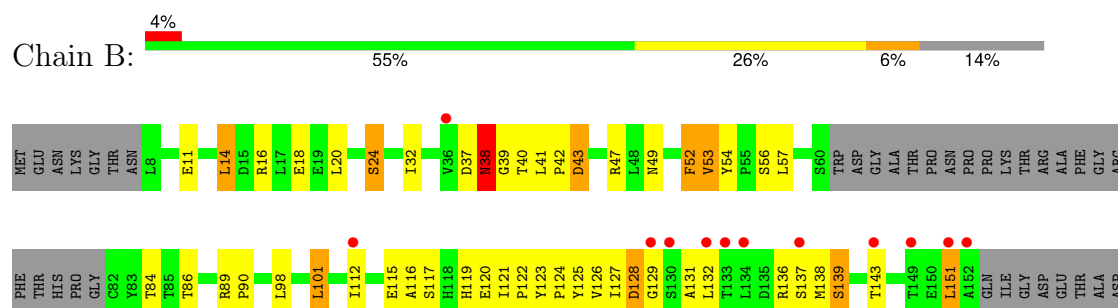
3 Residue-property plots [i](#)

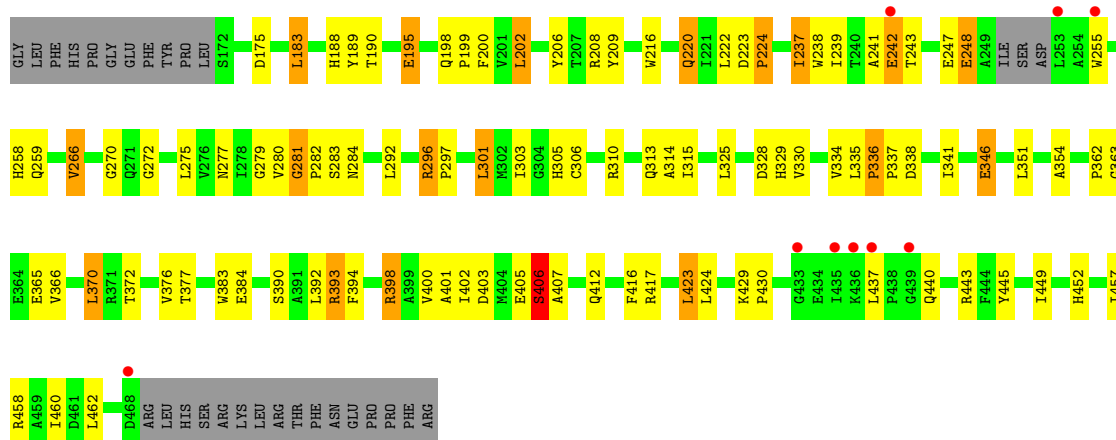
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: AMP nucleosidase

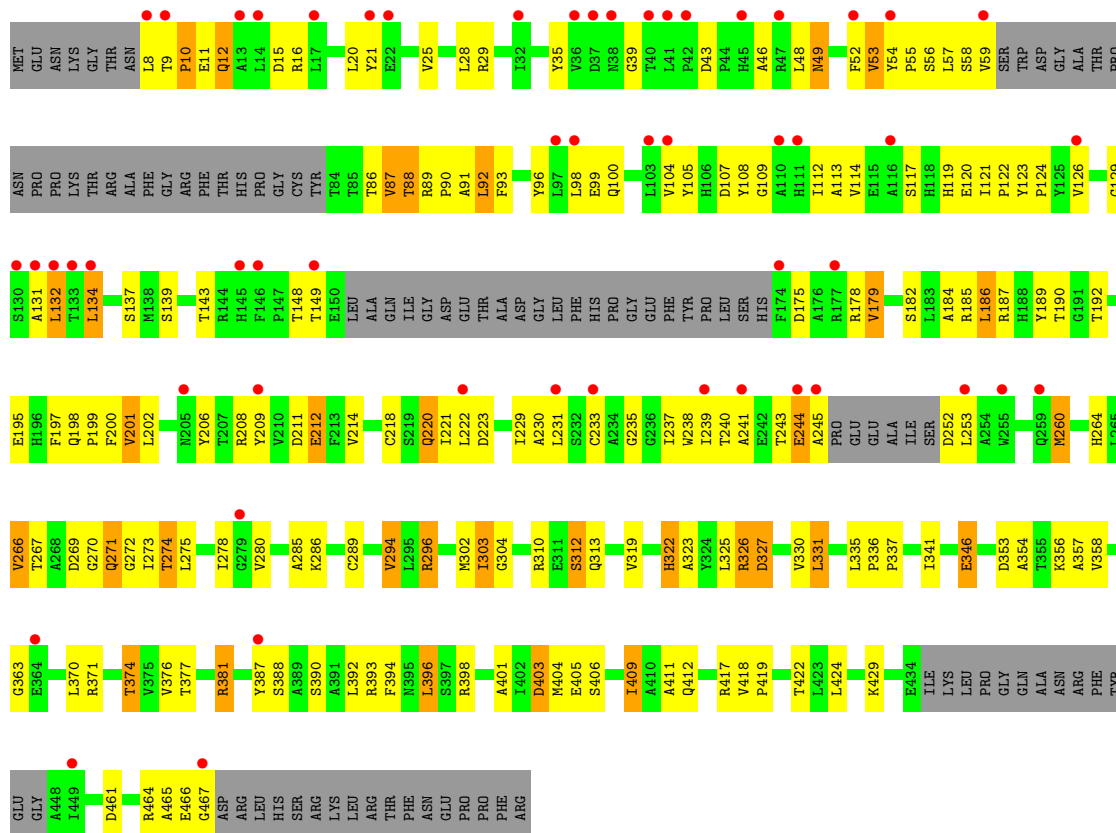


• Molecule 1: AMP nucleosidase





● Molecule 1: AMP nucleosidase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.49Å 170.28Å 204.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.07 – 2.64 45.07 – 2.64	Depositor EDS
% Data completeness (in resolution range)	93.0 (45.07-2.64) 93.1 (45.07-2.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.282 0.241 , 0.288	Depositor DCC
R_{free} test set	1381 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9415	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.48	0/3261	1.00	17/4453 (0.4%)
1	B	0.50	0/3320	1.02	15/4537 (0.3%)
1	C	0.45	0/3034	0.94	3/4154 (0.1%)
All	All	0.48	0/9615	0.99	35/13144 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	LYS	CA-C-N	8.78	129.32	119.32
1	A	429	LYS	C-N-CA	8.78	129.32	119.32
1	B	223	ASP	CA-C-N	8.34	130.27	119.84
1	B	223	ASP	C-N-CA	8.34	130.27	119.84
1	A	285	ALA	N-CA-C	-8.01	102.13	112.23
1	A	266	VAL	N-CA-C	7.22	118.36	110.21
1	B	449	ILE	N-CA-C	7.18	117.89	110.36
1	B	429	LYS	CA-C-N	7.02	127.33	119.32
1	B	429	LYS	C-N-CA	7.02	127.33	119.32
1	A	9	THR	CA-C-N	6.60	128.09	119.84
1	A	9	THR	C-N-CA	6.60	128.09	119.84
1	C	201	VAL	N-CA-C	6.53	118.00	108.53
1	A	450	SER	N-CA-C	-6.41	104.21	111.07
1	A	365	GLU	N-CA-C	-6.33	105.05	112.89
1	B	266	VAL	N-CA-C	6.04	116.64	110.05
1	B	325	LEU	N-CA-C	-5.97	98.80	108.41
1	A	435	ILE	N-CA-C	5.86	116.63	109.30
1	B	443	ARG	N-CA-C	5.69	117.16	111.07
1	A	133	THR	N-CA-C	5.57	117.72	110.43
1	B	189	TYR	N-CA-C	5.48	117.25	111.28
1	C	327	ASP	N-CA-C	-5.46	105.32	112.41
1	A	332	ASP	N-CA-C	5.42	117.19	111.28
1	A	201	VAL	N-CA-C	5.39	117.08	108.89
1	A	336	PRO	CA-C-N	5.26	124.97	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	PRO	C-N-CA	5.26	124.97	119.82
1	A	296	ARG	CA-C-N	5.14	125.42	119.92
1	A	296	ARG	C-N-CA	5.14	125.42	119.92
1	C	266	VAL	N-CA-C	5.12	117.77	110.09
1	B	281	GLY	CA-C-N	5.10	124.59	119.19
1	B	281	GLY	C-N-CA	5.10	124.59	119.19
1	B	336	PRO	CA-C-N	5.09	124.81	119.82
1	B	336	PRO	C-N-CA	5.09	124.81	119.82
1	A	252	ASP	N-CA-C	-5.08	106.30	113.20
1	B	137	SER	N-CA-C	-5.03	107.21	113.19
1	B	190	THR	N-CA-C	5.02	119.67	113.50

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	3182	0	3052	172	0
1	B	3240	0	3122	129	0
1	C	2964	0	2812	156	0
2	A	13	0	0	0	0
2	B	13	0	0	1	0
2	C	3	0	0	0	0
All	All	9415	0	8986	441	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 24.

All (441) 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:377:THR:HG21	1:B:407:ALA:H	1.05	1.09
1:B:393:ARG:HG3	1:B:393:ARG:HH11	1.18	1.07
1:B:151:LEU:HD12	1:B:151:LEU:H	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLN:HE21	1:B:272:GLY:H	1.12	0.96
1:A:151:LEU:H	1:A:151:LEU:HD22	1.34	0.92
1:C:29:ARG:HH12	1:C:129:GLY:HA3	1.32	0.92
1:B:14:LEU:HD13	1:B:98:LEU:HG	1.55	0.88
1:A:381:ARG:HH22	1:B:259:GLN:HE22	1.21	0.88
1:C:356:LYS:HD2	1:C:363:GLY:HA2	1.57	0.87
1:B:377:THR:HG21	1:B:407:ALA:N	1.90	0.87
1:C:330:VAL:HG13	1:C:331:LEU:HD22	1.59	0.84
1:A:202:LEU:HD13	1:A:460:ILE:HD11	1.59	0.84
1:A:8:LEU:HG	1:A:111:HIS:HB3	1.57	0.84
1:A:355:THR:O	1:A:359:SER:HB3	1.79	0.83
1:B:237:ILE:HD12	1:B:237:ILE:H	1.43	0.82
1:C:58:SER:HB3	1:C:113:ALA:HB3	1.61	0.82
1:C:123:TYR:O	1:C:126:VAL:HG12	1.81	0.80
1:C:240:THR:O	1:C:243:THR:HG22	1.82	0.79
1:A:205:ASN:H	1:A:205:ASN:HD22	1.30	0.79
1:B:198:GLN:HE22	1:B:270:GLY:HA2	1.47	0.79
1:C:202:LEU:HG	1:C:273:ILE:HD11	1.63	0.79
1:A:381:ARG:HH22	1:B:259:GLN:NE2	1.80	0.79
1:C:143:THR:HG23	1:C:148:THR:HG21	1.63	0.79
1:C:289:CYS:HB2	1:C:412:GLN:HG2	1.65	0.77
1:C:222:LEU:HD12	1:C:223:ASP:N	1.99	0.77
1:C:322:HIS:HE1	1:C:374:THR:HG22	1.50	0.77
1:A:296:ARG:HH11	1:A:296:ARG:HB3	1.50	0.77
1:B:398:ARG:HE	1:C:417:ARG:NH1	1.82	0.76
1:A:381:ARG:NH2	1:B:259:GLN:HE22	1.82	0.75
1:B:393:ARG:HH11	1:B:393:ARG:CG	1.96	0.75
1:B:237:ILE:HD12	1:B:237:ILE:N	2.02	0.75
1:B:41:LEU:HB2	1:B:42:PRO:HD2	1.69	0.74
1:B:209:TYR:OH	1:B:452:HIS:HD2	1.69	0.74
1:C:218:CYS:O	1:C:221:ILE:HG22	1.86	0.74
1:A:198:GLN:NE2	1:A:272:GLY:H	1.86	0.74
1:A:178:ARG:O	1:A:178:ARG:HD3	1.90	0.72
1:A:332:ASP:OD1	1:A:337:PRO:HG3	1.91	0.71
1:A:47:ARG:HA	1:A:51:LEU:HB2	1.71	0.70
1:A:205:ASN:H	1:A:205:ASN:ND2	1.89	0.70
1:C:275:LEU:C	1:C:275:LEU:HD23	2.16	0.70
1:A:134:LEU:N	1:A:134:LEU:HD12	2.07	0.69
1:C:390:SER:HB3	1:C:394:PHE:CE1	2.27	0.69
1:A:275:LEU:C	1:A:275:LEU:HD23	2.17	0.69
1:B:296:ARG:HE	1:B:296:ARG:HA	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:OD1	1:A:393:ARG:NH2	2.22	0.69
1:A:178:ARG:HD3	1:A:178:ARG:C	2.18	0.68
1:B:248:GLU:CD	1:B:248:GLU:H	2.02	0.68
1:A:34:ASP:O	1:A:38:ASN:HB3	1.94	0.68
1:A:28:LEU:HD23	1:A:126:VAL:HG11	1.75	0.68
1:A:198:GLN:HE21	1:A:272:GLY:H	1.39	0.67
1:C:132:LEU:HD21	1:C:134:LEU:HG	1.76	0.67
1:C:29:ARG:NH1	1:C:129:GLY:HA3	2.07	0.67
1:C:56:SER:HA	1:C:86:THR:HA	1.77	0.66
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.60	0.66
1:B:127:ILE:CG2	1:B:131:ALA:HB2	2.26	0.66
1:C:132:LEU:CD2	1:C:134:LEU:HG	2.26	0.66
1:C:197:PHE:HA	1:C:264:HIS:CD2	2.30	0.66
1:B:351:LEU:HB3	1:B:423:LEU:HD23	1.77	0.66
1:C:325:LEU:HB3	1:C:376:VAL:HG22	1.77	0.66
1:A:198:GLN:HE21	1:A:272:GLY:N	1.94	0.66
1:B:86:THR:HG21	1:B:119:HIS:HD2	1.60	0.66
1:C:89:ARG:N	1:C:90:PRO:HD3	2.11	0.65
1:C:198:GLN:HB3	1:C:272:GLY:O	1.96	0.65
1:B:255:TRP:HE1	1:B:277:ASN:ND2	1.94	0.65
1:A:296:ARG:HB3	1:A:296:ARG:NH1	2.11	0.65
1:C:370:LEU:HD12	1:C:371:ARG:H	1.62	0.64
1:A:89:ARG:HH11	1:A:89:ARG:HB3	1.62	0.64
1:C:285:ALA:HB1	1:C:409:ILE:HD12	1.79	0.64
1:A:123:TYR:O	1:A:126:VAL:HG22	1.98	0.64
1:C:8:LEU:HA	1:C:112:ILE:HB	1.80	0.64
1:C:132:LEU:HD22	1:C:134:LEU:H	1.62	0.64
1:B:377:THR:CG2	1:B:407:ALA:H	1.97	0.64
1:C:381:ARG:HD2	1:C:404:MET:SD	2.38	0.64
1:C:237:ILE:HD12	1:C:237:ILE:H	1.63	0.64
1:B:393:ARG:HG3	1:B:393:ARG:NH1	1.99	0.63
1:B:237:ILE:H	1:B:237:ILE:CD1	2.11	0.63
1:B:198:GLN:NE2	1:B:272:GLY:H	1.92	0.63
1:C:179:VAL:HA	1:C:294:VAL:HG21	1.80	0.62
1:B:362:PRO:HD2	1:B:365:GLU:OE2	2.00	0.62
1:C:392:LEU:HG	1:C:396:LEU:HD22	1.82	0.62
1:B:362:PRO:O	1:B:366:VAL:HG23	2.00	0.62
1:B:14:LEU:CD1	1:B:98:LEU:HG	2.28	0.62
1:C:231:LEU:HD12	1:C:264:HIS:O	1.99	0.62
1:A:209:TYR:CE1	1:A:449:ILE:HG23	2.34	0.62
1:A:325:LEU:HB3	1:A:376:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:HB3	1:A:147:PRO:HD2	1.82	0.62
1:A:199:PRO:HG2	1:A:200:PHE:CD1	2.34	0.62
1:C:202:LEU:HD22	1:C:303:ILE:HD13	1.83	0.61
1:C:289:CYS:CB	1:C:412:GLN:HG2	2.30	0.61
1:C:175:ASP:O	1:C:179:VAL:HG12	2.00	0.61
1:A:185:ARG:HD3	1:A:291:HIS:CE1	2.35	0.60
1:B:377:THR:HG22	1:B:403:ASP:OD2	2.00	0.60
1:A:151:LEU:H	1:A:151:LEU:CD2	2.13	0.60
1:A:344:ILE:HB	1:A:347:VAL:HG22	1.83	0.60
1:B:53:VAL:HG11	1:B:117:SER:O	2.01	0.60
1:B:101:LEU:HG	1:B:112:ILE:HD13	1.83	0.60
1:C:206:TYR:HB3	1:C:209:TYR:HD2	1.67	0.60
1:A:362:PRO:O	1:A:365:GLU:HB2	2.02	0.60
1:A:56:SER:HB2	1:A:117:SER:HB3	1.83	0.60
1:C:92:LEU:HD12	1:C:93:PHE:H	1.67	0.60
1:B:151:LEU:HD12	1:B:151:LEU:N	2.05	0.60
1:B:14:LEU:O	1:B:18:GLU:HG3	2.02	0.59
1:B:335:LEU:HD21	1:B:341:ILE:HD11	1.83	0.59
1:B:412:GLN:HE21	1:B:412:GLN:HA	1.67	0.59
1:C:21:TYR:O	1:C:25:VAL:HG23	2.01	0.59
1:A:206:TYR:HB3	1:A:209:TYR:CD1	2.38	0.59
1:A:324:TYR:OH	1:A:422:THR:HG23	2.02	0.59
1:A:59:VAL:HG12	1:A:112:ILE:HG22	1.84	0.59
1:A:16:ARG:HG3	1:A:16:ARG:HH11	1.69	0.58
1:A:183:LEU:HD22	1:A:194:VAL:HG11	1.85	0.58
1:A:291:HIS:O	1:A:294:VAL:HG22	2.03	0.58
1:A:347:VAL:HG21	1:A:420:TYR:O	2.04	0.58
1:C:296:ARG:HG3	1:C:296:ARG:HH11	1.69	0.58
1:C:370:LEU:HD12	1:C:371:ARG:N	2.17	0.58
1:C:187:ARG:HG3	1:C:192:THR:O	2.04	0.57
1:A:198:GLN:HE21	1:A:272:GLY:CA	2.17	0.57
1:B:202:LEU:HB3	1:B:275:LEU:HD23	1.84	0.57
1:C:206:TYR:HB3	1:C:209:TYR:CD2	2.38	0.57
1:A:57:LEU:HD23	1:A:57:LEU:C	2.29	0.57
1:A:436:LYS:HD3	1:A:442:ASN:OD1	2.04	0.57
1:B:127:ILE:O	1:B:128:ASP:HB2	2.05	0.57
1:C:465:ALA:C	1:C:467:GLY:H	2.13	0.57
1:B:199:PRO:HG2	1:B:200:PHE:CD1	2.40	0.57
1:A:275:LEU:HD23	1:A:276:VAL:N	2.20	0.57
1:A:102:ASN:C	1:A:104:VAL:H	2.13	0.56
1:B:151:LEU:H	1:B:151:LEU:CD1	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:HIS:O	1:B:258:HIS:HD2	1.88	0.56
1:C:260:MET:HE2	1:C:278:ILE:HA	1.87	0.56
1:B:121:ILE:N	1:B:121:ILE:HD12	2.21	0.56
1:A:430:PRO:O	1:B:151:LEU:HD11	2.06	0.56
1:B:398:ARG:NE	1:C:417:ARG:NH1	2.53	0.56
1:B:398:ARG:NE	1:C:417:ARG:CZ	2.69	0.56
1:A:282:PRO:HG3	1:A:379:ASP:HB3	1.87	0.56
1:C:240:THR:HG22	1:C:241:ALA:N	2.21	0.56
1:A:198:GLN:HE21	1:A:272:GLY:HA3	1.71	0.56
1:C:202:LEU:HB3	1:C:303:ILE:HD11	1.87	0.56
1:C:229:ILE:HG13	1:C:230:ALA:N	2.20	0.55
1:B:305:HIS:HB3	1:B:445:TYR:OH	2.07	0.55
1:B:412:GLN:HA	1:B:412:GLN:NE2	2.22	0.55
1:A:266:VAL:HG12	1:A:267:THR:N	2.22	0.55
1:A:151:LEU:HD12	1:B:384:GLU:HB3	1.90	0.55
1:C:98:LEU:C	1:C:100:GLN:H	2.15	0.55
1:B:437:LEU:O	1:B:440:GLN:HG3	2.08	0.54
1:C:92:LEU:HD12	1:C:93:PHE:N	2.22	0.54
1:C:286:LYS:HG3	1:C:412:GLN:NE2	2.21	0.54
1:A:200:PHE:HB3	1:A:460:ILE:HD13	1.89	0.54
1:A:444:PHE:N	1:A:444:PHE:CD1	2.74	0.54
1:B:376:VAL:HG12	1:B:401:ALA:O	2.06	0.54
1:B:198:GLN:HE21	1:B:272:GLY:N	1.93	0.54
1:A:209:TYR:CZ	1:A:449:ILE:HG23	2.42	0.54
1:C:20:LEU:CB	1:C:55:PRO:HB3	2.38	0.54
1:C:235:GLY:O	1:C:237:ILE:HD12	2.08	0.54
1:B:38:ASN:HB2	1:B:40:THR:HG23	1.90	0.54
1:C:25:VAL:O	1:C:29:ARG:HG3	2.07	0.54
1:C:59:VAL:HG11	1:C:104:VAL:HG11	1.89	0.54
1:C:266:VAL:HG12	1:C:267:THR:N	2.23	0.54
1:C:310:ARG:NH1	1:C:371:ARG:HH21	2.06	0.54
1:A:151:LEU:HD22	1:A:151:LEU:N	2.15	0.53
1:B:123:TYR:O	1:B:126:VAL:HG22	2.08	0.53
1:B:282:PRO:HB3	1:B:328:ASP:HB2	1.90	0.53
1:A:435:ILE:C	1:A:436:LYS:HG3	2.34	0.53
1:C:48:LEU:O	1:C:48:LEU:HD23	2.08	0.53
1:C:92:LEU:HD13	1:C:93:PHE:CD2	2.43	0.53
1:B:206:TYR:CE2	1:B:208:ARG:HB2	2.42	0.53
1:A:25:VAL:HG12	1:A:29:ARG:HH12	1.74	0.53
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.73	0.53
1:B:32:ILE:HD11	1:B:123:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLN:C	1:A:14:LEU:H	2.17	0.53
1:C:10:PRO:HG2	1:C:105:TYR:CG	2.44	0.53
1:C:20:LEU:HB2	1:C:55:PRO:HB3	1.91	0.53
1:A:446:GLU:C	1:A:448:ALA:H	2.17	0.53
1:C:322:HIS:CE1	1:C:374:THR:HG22	2.39	0.53
1:B:53:VAL:CG1	1:B:117:SER:H	2.22	0.53
1:C:235:GLY:C	1:C:237:ILE:HD12	2.33	0.53
1:A:21:TYR:OH	1:A:89:ARG:HD3	2.09	0.52
1:A:86:THR:HG23	1:A:176:ALA:H	1.73	0.52
1:A:259:GLN:HE22	1:B:280:VAL:HG11	1.73	0.52
1:B:127:ILE:HG23	1:B:131:ALA:HB2	1.91	0.52
1:C:220:GLN:HE21	1:C:220:GLN:N	2.07	0.52
1:C:211:ASP:O	1:C:214:VAL:HG12	2.10	0.52
1:C:237:ILE:HD12	1:C:237:ILE:N	2.25	0.52
1:A:199:PRO:HG2	1:A:200:PHE:CE1	2.44	0.52
1:B:216:TRP:CZ3	1:B:457:ILE:HD13	2.45	0.51
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.76	0.51
1:A:323:ALA:HB3	1:A:374:THR:HG22	1.92	0.51
1:C:221:ILE:HD11	1:C:239:ILE:O	2.10	0.51
1:B:241:ALA:C	1:B:243:THR:H	2.18	0.51
1:C:53:VAL:HA	1:C:119:HIS:O	2.11	0.51
1:A:310:ARG:O	1:A:429:LYS:NZ	2.43	0.51
1:B:123:TYR:CG	1:B:124:PRO:HD3	2.46	0.51
1:A:54:TYR:OH	1:A:180:ASP:OD2	2.25	0.51
1:A:8:LEU:O	1:A:12:GLN:HB3	2.10	0.50
1:A:9:THR:OG1	1:A:12:GLN:HB3	2.11	0.50
1:C:218:CYS:HA	1:C:221:ILE:HG22	1.93	0.50
1:A:231:LEU:HD12	1:A:264:HIS:O	2.11	0.50
1:A:350:ALA:HB2	1:A:463:LEU:HD13	1.92	0.50
1:C:310:ARG:HG3	1:C:310:ARG:HH11	1.76	0.50
1:A:173:HIS:O	1:A:174:PHE:HB2	2.11	0.50
1:B:417:ARG:HH11	1:C:398:ARG:NH1	2.10	0.50
1:C:56:SER:HB3	1:C:117:SER:HB3	1.93	0.50
1:A:435:ILE:O	1:A:436:LYS:HG3	2.11	0.50
1:A:444:PHE:HD1	1:A:444:PHE:H	1.60	0.50
1:A:192:THR:HG22	1:A:234:ALA:HA	1.93	0.50
1:A:428:ASP:OD2	1:A:430:PRO:HG3	2.12	0.50
1:B:16:ARG:O	1:B:20:LEU:HB2	2.11	0.49
1:B:122:PRO:HD2	1:B:125:TYR:HD2	1.77	0.49
1:A:209:TYR:CE1	1:A:449:ILE:HD12	2.47	0.49
1:C:123:TYR:N	1:C:124:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:TYR:CD2	1:C:208:ARG:HB2	2.47	0.49
1:B:354:ALA:HB1	1:B:458:ARG:HB3	1.94	0.49
1:C:175:ASP:OD1	1:C:175:ASP:C	2.56	0.49
1:A:458:ARG:O	1:A:461:ASP:HB2	2.12	0.49
1:B:216:TRP:O	1:B:220:GLN:HB2	2.12	0.49
1:B:390:SER:HB3	1:B:394:PHE:CE1	2.47	0.49
1:C:253:LEU:HG	1:C:253:LEU:O	2.13	0.49
1:A:212:GLU:O	1:A:215:ARG:HB3	2.13	0.49
1:A:151:LEU:HD21	1:B:430:PRO:O	2.13	0.49
1:B:247:GLU:H	1:B:247:GLU:CD	2.21	0.49
1:A:310:ARG:NH1	1:A:400:VAL:HG23	2.27	0.49
1:C:346:GLU:CD	1:C:346:GLU:H	2.20	0.49
1:C:89:ARG:O	1:C:92:LEU:HD12	2.13	0.48
1:C:390:SER:HB3	1:C:394:PHE:CZ	2.47	0.48
1:A:20:LEU:HD13	1:A:115:GLU:O	2.13	0.48
1:A:436:LYS:HZ2	1:A:442:ASN:CG	2.21	0.48
1:C:233:CYS:HB2	1:C:237:ILE:HB	1.96	0.48
1:A:251:SER:C	1:A:253:LEU:H	2.22	0.48
1:A:325:LEU:HD23	1:A:376:VAL:HG22	1.95	0.48
1:A:436:LYS:HZ2	1:A:442:ASN:ND2	2.12	0.48
1:B:127:ILE:O	1:B:128:ASP:CB	2.62	0.48
1:C:12:GLN:O	1:C:15:ASP:N	2.47	0.48
1:C:198:GLN:HB2	1:C:274:THR:HG22	1.95	0.48
1:B:11:GLU:HB2	2:B:487:HOH:O	2.14	0.48
1:B:127:ILE:HG21	1:B:131:ALA:HB2	1.94	0.48
1:A:151:LEU:O	1:A:153:GLN:HG2	2.14	0.48
1:A:386:ARG:HD2	1:B:334:VAL:CG1	2.43	0.47
1:C:182:SER:O	1:C:186:LEU:HB2	2.14	0.47
1:C:221:ILE:HD13	1:C:239:ILE:HG22	1.96	0.47
1:C:465:ALA:C	1:C:467:GLY:N	2.72	0.47
1:B:437:LEU:HB2	1:B:440:GLN:OE1	2.15	0.47
1:C:86:THR:HG21	1:C:119:HIS:HD2	1.78	0.47
1:C:137:SER:C	1:C:139:SER:H	2.20	0.47
1:C:285:ALA:HB1	1:C:409:ILE:CD1	2.43	0.47
1:A:27:ALA:HB1	1:A:51:LEU:CD2	2.44	0.47
1:B:383:TRP:CE2	1:B:402:ILE:HD13	2.49	0.47
1:C:28:LEU:HA	1:C:52:PHE:CE2	2.49	0.47
1:A:189:TYR:CD1	1:A:260:MET:HE3	2.49	0.47
1:B:175:ASP:OD2	1:B:175:ASP:C	2.56	0.47
1:C:187:ARG:O	1:C:190:THR:O	2.33	0.47
1:A:16:ARG:HB2	1:A:114:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:O	1:A:23:GLN:HB2	2.14	0.47
1:A:41:LEU:N	1:A:41:LEU:HD22	2.29	0.47
1:A:214:VAL:HG11	1:A:249:ALA:HB3	1.96	0.47
1:A:315:ILE:HG13	1:A:436:LYS:HE3	1.97	0.47
1:A:358:VAL:CG2	1:A:458:ARG:HG3	2.44	0.47
1:C:322:HIS:ND1	1:C:322:HIS:C	2.72	0.47
1:C:412:GLN:OE1	1:C:412:GLN:HA	2.15	0.47
1:A:20:LEU:O	1:A:23:GLN:HB3	2.14	0.47
1:A:32:ILE:O	1:A:36:VAL:HG23	2.14	0.47
1:C:218:CYS:HA	1:C:221:ILE:CG2	2.45	0.47
1:C:237:ILE:HG22	1:C:238:TRP:N	2.29	0.47
1:A:305:HIS:HB3	1:A:445:TYR:OH	2.14	0.47
1:C:43:ASP:HB3	1:C:46:ALA:HB2	1.97	0.47
1:C:273:ILE:HG13	1:C:274:THR:N	2.29	0.47
1:A:13:ALA:HA	1:A:114:VAL:HG11	1.96	0.47
1:A:206:TYR:HB3	1:A:209:TYR:HD1	1.79	0.47
1:A:261:PRO:HB2	1:A:263:TRP:CH2	2.50	0.47
1:A:434:GLU:CA	1:B:143:THR:HG21	2.44	0.47
1:B:338:ASP:OD2	1:C:393:ARG:NH2	2.47	0.47
1:C:275:LEU:C	1:C:275:LEU:CD2	2.88	0.47
1:C:461:ASP:HA	1:C:464:ARG:NH1	2.30	0.47
1:A:327:ASP:CG	1:A:393:ARG:HH21	2.20	0.46
1:B:202:LEU:HB3	1:B:275:LEU:CD2	2.45	0.46
1:C:43:ASP:HB3	1:C:46:ALA:CB	2.45	0.46
1:C:327:ASP:CG	1:C:393:ARG:HH12	2.22	0.46
1:B:37:ASP:C	1:B:39:GLY:H	2.23	0.46
1:A:84:THR:HG23	1:A:84:THR:O	2.16	0.46
1:A:94:ARG:HG3	1:A:94:ARG:HH11	1.81	0.46
1:A:132:LEU:HD23	1:A:132:LEU:C	2.40	0.46
1:A:198:GLN:HB2	1:A:274:THR:HG22	1.96	0.46
1:A:332:ASP:OD1	1:A:337:PRO:CG	2.61	0.46
1:C:122:PRO:C	1:C:124:PRO:HD2	2.40	0.46
1:A:58:SER:OG	1:A:84:THR:HB	2.15	0.46
1:C:270:GLY:O	1:C:271:GLN:NE2	2.49	0.46
1:A:205:ASN:ND2	1:A:205:ASN:N	2.50	0.46
1:B:198:GLN:HE22	1:B:270:GLY:CA	2.24	0.46
1:A:89:ARG:HB3	1:A:89:ARG:NH1	2.27	0.46
1:B:136:ARG:C	1:B:138:MET:H	2.22	0.46
1:B:195:GLU:CD	1:B:195:GLU:H	2.22	0.46
1:B:310:ARG:HB2	1:B:313:GLN:HG3	1.97	0.46
1:B:393:ARG:CG	1:B:393:ARG:NH1	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:HH11	1:A:386:ARG:HG2	1.80	0.45
1:A:24:SER:CB	1:A:52:PHE:HA	2.46	0.45
1:A:275:LEU:C	1:A:275:LEU:CD2	2.88	0.45
1:B:47:ARG:HG2	1:B:52:PHE:CE1	2.52	0.45
1:B:138:MET:O	1:B:139:SER:C	2.59	0.45
1:C:16:ARG:HD2	1:C:114:VAL:HG12	1.98	0.45
1:A:192:THR:CG2	1:A:234:ALA:HA	2.46	0.45
1:C:53:VAL:HG11	1:C:117:SER:O	2.16	0.45
1:A:451:GLU:O	1:A:455:ILE:HG13	2.17	0.45
1:A:57:LEU:HD23	1:A:57:LEU:O	2.16	0.45
1:A:259:GLN:O	1:A:260:MET:HG3	2.16	0.45
1:A:14:LEU:HG	1:A:94:ARG:NH1	2.31	0.45
1:B:202:LEU:HD13	1:B:460:ILE:CD1	2.47	0.45
1:A:10:PRO:C	1:A:12:GLN:N	2.75	0.45
1:B:43:ASP:OD1	1:B:43:ASP:N	2.48	0.45
1:B:346:GLU:CD	1:B:346:GLU:H	2.24	0.45
1:C:199:PRO:HG2	1:C:200:PHE:CD1	2.52	0.45
1:C:313:GLN:HG3	1:C:429:LYS:NZ	2.32	0.45
1:A:305:HIS:CD2	1:A:438:PRO:HG2	2.52	0.45
1:A:443:ARG:HG2	1:A:443:ARG:HH11	1.83	0.45
1:A:381:ARG:HB2	1:A:404:MET:SD	2.57	0.44
1:C:319:VAL:HG21	1:C:401:ALA:HB2	1.99	0.44
1:C:325:LEU:HD12	1:C:325:LEU:HA	1.84	0.44
1:A:21:TYR:CD2	1:A:90:PRO:HD2	2.53	0.44
1:A:104:VAL:O	1:A:108:TYR:HB2	2.18	0.44
1:C:35:TYR:O	1:C:39:GLY:HA2	2.16	0.44
1:C:313:GLN:HG3	1:C:429:LYS:HZ3	1.82	0.44
1:C:201:VAL:HG22	1:C:274:THR:HG23	1.99	0.44
1:A:123:TYR:CG	1:A:124:PRO:HD3	2.53	0.44
1:A:190:THR:HA	1:A:260:MET:O	2.17	0.44
1:C:304:GLY:O	1:C:424:LEU:HA	2.18	0.44
1:C:418:VAL:O	1:C:419:PRO:C	2.60	0.44
1:A:201:VAL:HA	1:A:274:THR:HG23	2.00	0.44
1:B:54:TYR:CE2	1:B:121:ILE:HG13	2.53	0.44
1:B:241:ALA:O	1:B:243:THR:N	2.46	0.44
1:A:436:LYS:NZ	1:A:442:ASN:ND2	2.66	0.44
1:C:394:PHE:N	1:C:394:PHE:CD1	2.85	0.44
1:A:259:GLN:NE2	1:B:280:VAL:HG11	2.33	0.44
1:C:336:PRO:HA	1:C:337:PRO:HD3	1.88	0.43
1:A:12:GLN:O	1:A:13:ALA:HB3	2.16	0.43
1:A:44:PRO:O	1:A:48:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD12	1:B:121:ILE:H	1.82	0.43
1:C:89:ARG:N	1:C:90:PRO:CD	2.80	0.43
1:C:137:SER:C	1:C:139:SER:N	2.76	0.43
1:B:124:PRO:HA	1:B:127:ILE:HD12	1.99	0.43
1:B:314:ALA:O	1:B:315:ILE:C	2.61	0.43
1:C:394:PHE:N	1:C:394:PHE:HD1	2.17	0.43
1:C:16:ARG:CZ	1:C:20:LEU:HD21	2.48	0.43
1:C:296:ARG:HH11	1:C:296:ARG:CG	2.31	0.43
1:C:358:VAL:O	1:C:358:VAL:HG12	2.18	0.43
1:B:437:LEU:H	1:B:440:GLN:CD	2.25	0.43
1:C:326:ARG:HD3	1:C:341:ILE:HD12	2.01	0.43
1:A:9:THR:OG1	1:A:12:GLN:CB	2.67	0.43
1:A:16:ARG:HG3	1:A:16:ARG:NH1	2.34	0.43
1:A:233:CYS:HB2	1:A:237:ILE:HG12	2.00	0.43
1:C:9:THR:HB	1:C:12:GLN:OE1	2.19	0.43
1:C:200:PHE:O	1:C:273:ILE:HD12	2.19	0.43
1:A:329:HIS:HA	1:A:332:ASP:OD2	2.18	0.43
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.89	0.43
1:B:328:ASP:O	1:B:330:VAL:N	2.50	0.43
1:C:202:LEU:HD22	1:C:303:ILE:CD1	2.47	0.43
1:A:330:VAL:HG13	1:A:331:LEU:HG	2.01	0.43
1:A:102:ASN:C	1:A:104:VAL:N	2.77	0.42
1:C:55:PRO:HG2	1:C:87:VAL:HG22	2.00	0.42
1:B:437:LEU:HD23	1:B:440:GLN:OE1	2.19	0.42
1:A:191:GLY:O	1:A:234:ALA:O	2.36	0.42
1:C:54:TYR:CE2	1:C:88:THR:HB	2.54	0.42
1:A:208:ARG:O	1:A:211:ASP:HB2	2.20	0.42
1:A:296:ARG:HH11	1:A:296:ARG:CB	2.28	0.42
1:A:107:ASP:O	1:A:108:TYR:CD1	2.72	0.42
1:A:175:ASP:O	1:A:176:ALA:C	2.63	0.42
1:A:200:PHE:CZ	1:A:464:ARG:HG3	2.54	0.42
1:B:306:CYS:HB3	1:B:424:LEU:HD13	2.01	0.42
1:C:20:LEU:HB3	1:C:55:PRO:HB3	2.02	0.42
1:C:49:ASN:HD22	1:C:49:ASN:HA	1.66	0.42
1:C:189:TYR:HB3	1:C:260:MET:HG3	2.01	0.42
1:B:47:ARG:HH21	1:B:120:GLU:CD	2.27	0.42
1:A:440:GLN:O	1:A:441:ALA:HB3	2.20	0.42
1:B:56:SER:HB2	1:B:117:SER:HB3	2.01	0.42
1:B:238:TRP:O	1:B:239:ILE:HD13	2.19	0.42
1:B:403:ASP:OD1	1:B:406:SER:HB2	2.20	0.42
1:B:416:PHE:C	1:B:417:ARG:HG2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:CB	1:A:376:VAL:HG22	2.47	0.42
1:B:89:ARG:N	1:B:90:PRO:HD3	2.34	0.42
1:B:136:ARG:C	1:B:138:MET:N	2.76	0.42
1:B:301:LEU:HB3	1:B:303:ILE:CD1	2.50	0.42
1:C:187:ARG:HG2	1:C:187:ARG:HH11	1.85	0.42
1:A:112:ILE:O	1:A:112:ILE:HG13	2.20	0.42
1:B:115:GLU:O	1:B:116:ALA:C	2.63	0.42
1:B:132:LEU:HD12	1:B:132:LEU:N	2.35	0.42
1:A:132:LEU:HD23	1:A:132:LEU:O	2.20	0.41
1:A:322:HIS:CD2	1:A:373:GLY:C	2.98	0.41
1:A:443:ARG:HG2	1:A:443:ARG:NH1	2.35	0.41
1:C:244:GLU:CD	1:C:245:ALA:H	2.28	0.41
1:A:247:GLU:N	1:A:247:GLU:OE1	2.53	0.41
1:B:41:LEU:CB	1:B:42:PRO:HD2	2.46	0.41
1:B:417:ARG:NH1	1:C:398:ARG:NH1	2.68	0.41
1:C:201:VAL:HG22	1:C:274:THR:CG2	2.50	0.41
1:C:260:MET:HE2	1:C:260:MET:HB3	1.94	0.41
1:B:377:THR:HA	1:B:403:ASP:O	2.20	0.41
1:C:302:MET:HB3	1:C:422:THR:HG22	2.02	0.41
1:A:182:SER:OG	1:A:291:HIS:HD2	2.03	0.41
1:B:296:ARG:N	1:B:297:PRO:HD3	2.35	0.41
1:C:221:ILE:HD11	1:C:230:ALA:HA	2.02	0.41
1:C:323:ALA:HB3	1:C:374:THR:HB	2.02	0.41
1:C:353:ASP:O	1:C:354:ALA:C	2.62	0.41
1:A:134:LEU:N	1:A:134:LEU:CD1	2.79	0.41
1:B:41:LEU:HD12	1:B:41:LEU:C	2.46	0.41
1:C:178:ARG:NH1	1:C:182:SER:OG	2.54	0.41
1:A:89:ARG:N	1:A:90:PRO:CD	2.83	0.41
1:A:205:ASN:HD22	1:A:205:ASN:N	1.96	0.41
1:A:446:GLU:HA	1:A:449:ILE:HG12	2.02	0.41
1:B:255:TRP:HE1	1:B:277:ASN:HD22	1.64	0.41
1:C:54:TYR:CE1	1:C:121:ILE:HA	2.55	0.41
1:C:132:LEU:HD22	1:C:134:LEU:HG	2.02	0.41
1:C:266:VAL:HG12	1:C:267:THR:H	1.85	0.41
1:A:135:ASP:OD1	1:A:138:MET:HG2	2.21	0.41
1:A:202:LEU:CD1	1:A:460:ILE:HD11	2.40	0.41
1:A:280:VAL:HA	1:A:405:GLU:OE2	2.21	0.41
1:A:336:PRO:HA	1:A:337:PRO:HD3	1.82	0.41
1:B:47:ARG:C	1:B:49:ASN:N	2.79	0.41
1:C:240:THR:HG22	1:C:241:ALA:H	1.86	0.41
1:C:341:ILE:CD1	1:C:411:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:N	1:A:8:LEU:HD12	2.35	0.41
1:A:10:PRO:O	1:A:12:GLN:O	2.39	0.41
1:A:185:ARG:HD3	1:A:291:HIS:NE2	2.36	0.41
1:A:260:MET:HG2	1:A:278:ILE:HA	2.03	0.41
1:B:202:LEU:HG	1:B:303:ILE:HD13	2.03	0.41
1:C:53:VAL:HA	1:C:120:GLU:HA	2.02	0.41
1:C:96:TYR:O	1:C:100:GLN:HB2	2.20	0.41
1:C:208:ARG:O	1:C:212:GLU:HB2	2.21	0.41
1:A:196:HIS:CD2	1:A:238:TRP:HE1	2.39	0.41
1:B:281:GLY:HA2	1:B:282:PRO:HD3	1.86	0.41
1:B:115:GLU:OE2	1:B:116:ALA:O	2.39	0.40
1:B:259:GLN:NE2	1:B:284:ASN:OD1	2.52	0.40
1:C:12:GLN:O	1:C:16:ARG:N	2.48	0.40
1:A:206:TYR:HD1	1:A:209:TYR:HE1	1.69	0.40
1:B:24:SER:OG	1:B:53:VAL:N	2.55	0.40
1:B:394:PHE:N	1:B:394:PHE:CD1	2.89	0.40
1:C:269:ASP:OD2	1:C:271:GLN:HB2	2.21	0.40
1:A:47:ARG:CA	1:A:51:LEU:HB2	2.48	0.40
1:A:201:VAL:HG23	1:A:202:LEU:N	2.36	0.40
1:B:328:ASP:C	1:B:330:VAL:H	2.30	0.40
1:B:336:PRO:HA	1:B:337:PRO:HD3	1.79	0.40
1:B:370:LEU:HD13	1:B:370:LEU:O	2.19	0.40
1:C:325:LEU:CB	1:C:376:VAL:HG22	2.50	0.40
1:C:387:TYR:O	1:C:388:SER:C	2.63	0.40
1:A:32:ILE:CD1	1:A:123:TYR:HB2	2.50	0.40
1:B:200:PHE:HB3	1:B:460:ILE:HD13	2.04	0.40
1:C:98:LEU:O	1:C:100:GLN:N	2.55	0.40
1:C:377:THR:HA	1:C:403:ASP:O	2.20	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	403/484 (83%)	348 (86%)	47 (12%)	8 (2%)	6	8
1	B	410/484 (85%)	375 (92%)	25 (6%)	10 (2%)	4	6
1	C	384/484 (79%)	331 (86%)	38 (10%)	15 (4%)	2	2
All	All	1197/1452 (82%)	1054 (88%)	110 (9%)	33 (3%)	4	4

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	B	128	ASP
1	B	224	PRO
1	C	11	GLU
1	C	108	TYR
1	C	134	LEU
1	A	38	ASN
1	C	91	ALA
1	C	99	GLU
1	C	107	ASP
1	C	109	GLY
1	A	10	PRO
1	A	215	ARG
1	B	242	GLU
1	B	363	GLY
1	B	406	SER
1	A	248	GLU
1	A	436	LYS
1	B	38	ASN
1	B	139	SER
1	B	279	GLY
1	C	131	ALA
1	C	184	ALA
1	C	312	SER
1	C	357	ALA
1	C	10	PRO
1	C	53	VAL
1	C	466	GLU
1	B	329	HIS
1	C	406	SER
1	A	9	THR
1	B	129	GLY
1	A	299	VAL

5.3.2 Protein sidechains ⓘ

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	327/403 (81%)	292 (89%)	35 (11%)	6	9
1	B	337/403 (84%)	302 (90%)	35 (10%)	7	9
1	C	297/403 (74%)	262 (88%)	35 (12%)	5	6
All	All	961/1209 (80%)	856 (89%)	105 (11%)	6	8

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	52	PHE
1	A	89	ARG
1	A	134	LEU
1	A	150	GLU
1	A	151	LEU
1	A	173	HIS
1	A	175	ASP
1	A	178	ARG
1	A	201	VAL
1	A	202	LEU
1	A	205	ASN
1	A	220	GLN
1	A	237	ILE
1	A	238	TRP
1	A	247	GLU
1	A	274	THR
1	A	280	VAL
1	A	292	LEU
1	A	296	ARG
1	A	298	ASP
1	A	309	LEU
1	A	351	LEU
1	A	359	SER
1	A	365	GLU
1	A	366	VAL

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Mol	Chain	Res	Type
1	A	374	THR
1	A	400	VAL
1	A	422	THR
1	A	431	LEU
1	A	436	LYS
1	A	444	PHE
1	A	450	SER
1	A	462	LEU
1	A	463	LEU
1	B	14	LEU
1	B	24	SER
1	B	38	ASN
1	B	43	ASP
1	B	52	PHE
1	B	53	VAL
1	B	57	LEU
1	B	84	THR
1	B	101	LEU
1	B	151	LEU
1	B	183	LEU
1	B	195	GLU
1	B	202	LEU
1	B	220	GLN
1	B	222	LEU
1	B	224	PRO
1	B	237	ILE
1	B	242	GLU
1	B	248	GLU
1	B	266	VAL
1	B	283	SER
1	B	292	LEU
1	B	296	ARG
1	B	301	LEU
1	B	346	GLU
1	B	370	LEU
1	B	372	THR
1	B	392	LEU
1	B	393	ARG
1	B	398	ARG
1	B	400	VAL
1	B	405	GLU
1	B	406	SER

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Mol	Chain	Res	Type
1	B	423	LEU
1	B	462	LEU
1	C	12	GLN
1	C	49	ASN
1	C	57	LEU
1	C	87	VAL
1	C	88	THR
1	C	92	LEU
1	C	132	LEU
1	C	149	THR
1	C	179	VAL
1	C	185	ARG
1	C	186	LEU
1	C	195	GLU
1	C	212	GLU
1	C	220	GLN
1	C	244	GLU
1	C	252	ASP
1	C	260	MET
1	C	271	GLN
1	C	274	THR
1	C	280	VAL
1	C	294	VAL
1	C	296	ARG
1	C	303	ILE
1	C	312	SER
1	C	322	HIS
1	C	326	ARG
1	C	331	LEU
1	C	335	LEU
1	C	346	GLU
1	C	374	THR
1	C	381	ARG
1	C	396	LEU
1	C	403	ASP
1	C	405	GLU
1	C	409	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN

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Mol	Chain	Res	Type
1	A	49	ASN
1	A	118	HIS
1	A	145	HIS
1	A	173	HIS
1	A	198	GLN
1	A	205	ASN
1	A	220	GLN
1	A	259	GLN
1	A	271	GLN
1	A	291	HIS
1	A	348	GLN
1	A	382	ASN
1	A	432	HIS
1	A	442	ASN
1	B	26	ASN
1	B	45	HIS
1	B	49	ASN
1	B	119	HIS
1	B	198	GLN
1	B	220	GLN
1	B	258	HIS
1	B	259	GLN
1	B	277	ASN
1	B	368	GLN
1	B	382	ASN
1	B	412	GLN
1	B	442	ASN
1	B	452	HIS
1	C	26	ASN
1	C	49	ASN
1	C	119	HIS
1	C	188	HIS
1	C	220	GLN
1	C	264	HIS
1	C	271	GLN
1	C	291	HIS
1	C	395	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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, 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	411/484 (84%)	0.71	44 (10%) 11 9	37, 72, 118, 129	0
1	B	418/484 (86%)	0.34	21 (5%) 34 28	38, 60, 103, 115	0
1	C	394/484 (81%)	0.85	54 (13%) 6 5	43, 82, 119, 124	0
All	All	1223/1452 (84%)	0.63	119 (9%) 13 10	37, 69, 116, 129	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	ILE	8.2
1	C	245	ALA	8.1
1	A	437	LEU	7.5
1	C	133	THR	6.4
1	B	132	LEU	6.3
1	C	8	LEU	6.3
1	C	132	LEU	5.6
1	B	130	SER	5.6
1	A	8	LEU	5.0
1	A	133	THR	4.9
1	A	436	LYS	4.6
1	B	152	ALA	4.3
1	A	110	ALA	4.2
1	A	112	ILE	4.1
1	C	130	SER	4.1
1	B	129	GLY	4.0
1	A	438	PRO	4.0
1	A	127	ILE	4.0
1	B	134	LEU	3.9
1	A	252	ASP	3.9
1	A	132	LEU	3.8
1	C	146	PHE	3.8
1	B	433	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	363	GLY	3.7
1	C	110	ALA	3.6
1	C	131	ALA	3.6
1	C	17	LEU	3.6
1	C	41	LEU	3.6
1	A	442	ASN	3.6
1	C	255	TRP	3.6
1	C	467	GLY	3.6
1	C	449	ILE	3.5
1	B	133	THR	3.4
1	A	255	TRP	3.3
1	A	59	VAL	3.3
1	A	131	ALA	3.3
1	A	104	VAL	3.3
1	A	221	ILE	3.3
1	C	103	LEU	3.3
1	C	134	LEU	3.3
1	C	241	ALA	3.3
1	B	436	LYS	3.2
1	C	233	CYS	3.2
1	B	137	SER	3.2
1	C	149	THR	3.2
1	B	435	ILE	3.1
1	A	440	GLN	3.1
1	A	250	ILE	3.1
1	A	249	ALA	3.1
1	B	253	LEU	3.1
1	C	14	LEU	3.1
1	A	445	TYR	3.0
1	C	42	PRO	3.0
1	C	40	THR	3.0
1	B	242	GLU	3.0
1	C	38	ASN	3.0
1	C	21	TYR	3.0
1	C	231	LEU	2.9
1	C	37	ASP	2.9
1	C	116	ALA	2.9
1	C	47	ARG	2.9
1	A	441	ALA	2.9
1	B	439	GLY	2.8
1	C	36	VAL	2.8
1	C	104	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	22	GLU	2.8
1	B	437	LEU	2.8
1	A	151	LEU	2.7
1	C	97	LEU	2.7
1	C	145	HIS	2.7
1	A	111	HIS	2.7
1	B	143	THR	2.7
1	B	468	ASP	2.7
1	A	113	ALA	2.6
1	C	239	ILE	2.6
1	B	151	LEU	2.6
1	B	255	TRP	2.5
1	A	11	GLU	2.5
1	A	152	ALA	2.5
1	A	238	TRP	2.5
1	C	54	TYR	2.4
1	C	222	LEU	2.4
1	C	253	LEU	2.4
1	C	205	ASN	2.4
1	A	17	LEU	2.3
1	A	239	ILE	2.3
1	B	149	THR	2.3
1	C	111	HIS	2.3
1	C	52	PHE	2.3
1	A	225	ASP	2.3
1	A	149	THR	2.3
1	C	45	HIS	2.2
1	C	209	TYR	2.2
1	A	130	SER	2.2
1	A	320	LEU	2.2
1	C	98	LEU	2.2
1	A	444	PHE	2.2
1	C	174	PHE	2.2
1	A	224	PRO	2.2
1	A	58	SER	2.2
1	A	32	ILE	2.2
1	B	36	VAL	2.2
1	C	13	ALA	2.1
1	C	244	GLU	2.1
1	C	9	THR	2.1
1	C	364	GLU	2.1
1	C	259	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	2.1
1	A	366	VAL	2.1
1	B	112	ILE	2.1
1	C	59	VAL	2.1
1	A	53	VAL	2.1
1	C	126	VAL	2.1
1	A	52	PHE	2.1
1	C	387	TYR	2.0
1	C	177	ARG	2.0
1	A	439	GLY	2.0
1	C	32	ILE	2.0
1	C	279	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 oligosaccharides 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.