Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 11:36 am BST

PDB ID	:	2W45
Title	:	Epstein-Barr virus alkaline nuclease
Authors	:	Buisson, M.; Geoui, T.; Flot, D.; Tarbouriech, N.; Burmeister, W.P.
Deposited on	:	2008-11-21
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

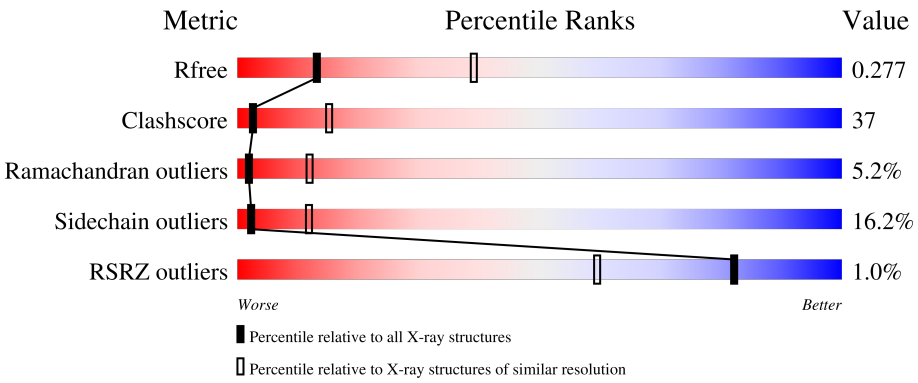
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	470	
1	B	470	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7009 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 ALKALINE EXONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	449	3539	2257	595	665	22	0	0	0
1	B	437	3446	2201	579	644	22	0	0	0

- Molecule 2 is water.

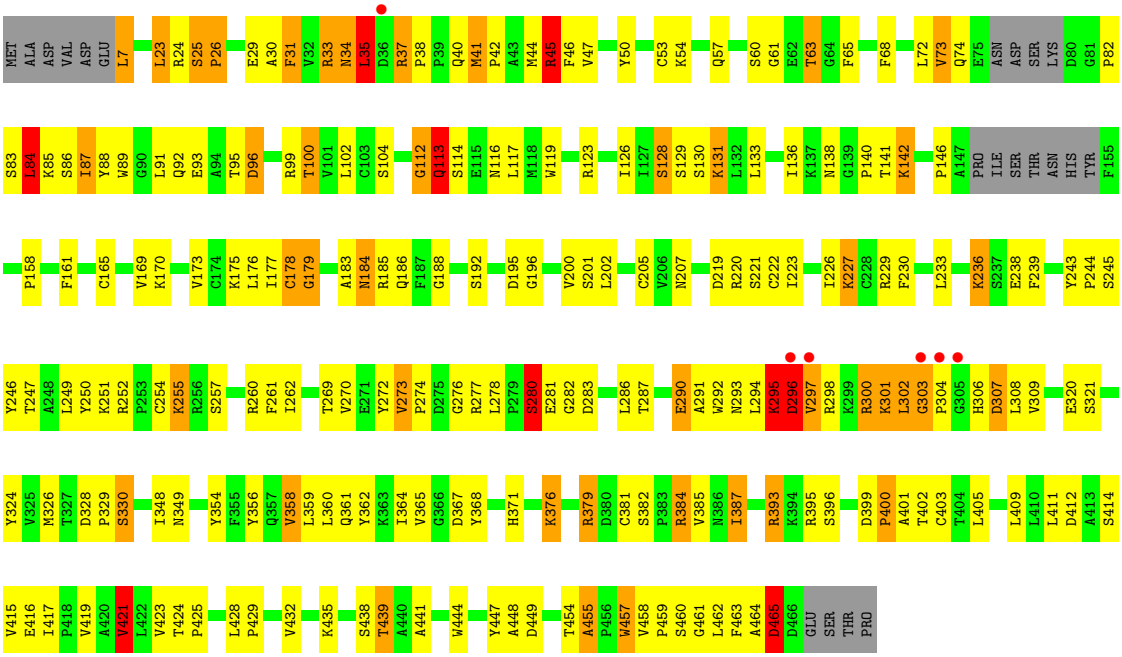
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	10	10	10	0	0
2	B	14	14	14	0	0

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.

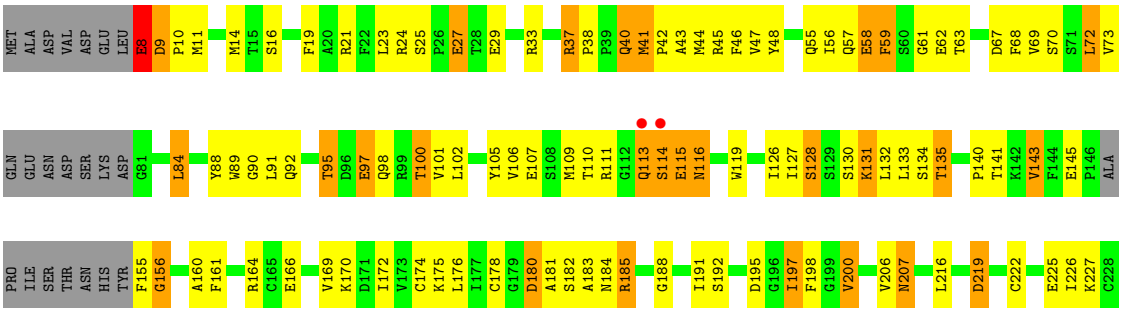
• Molecule 1: ALKALINE EXONUCLEASE

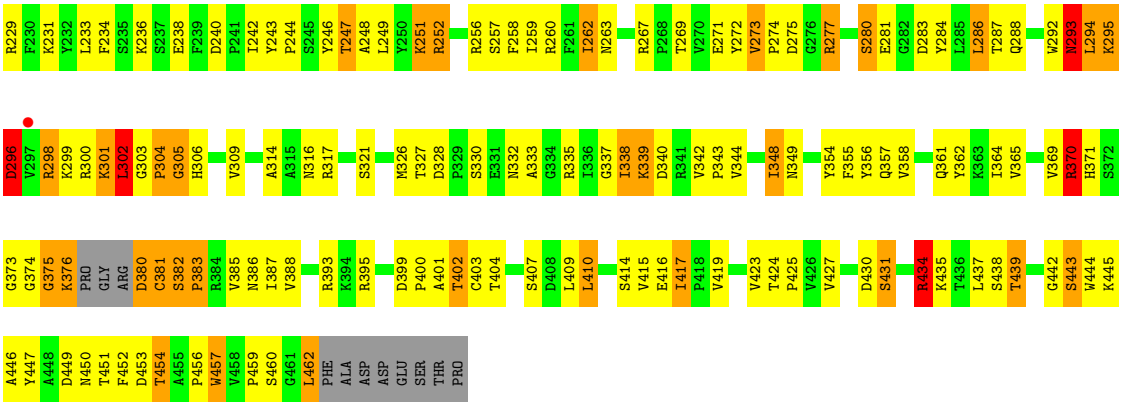
Chain A:



• Molecule 1: ALKALINE EXONUCLEASE

Chain B:




R229 F230 K231 Y232 L233 F234 S235 K236 S237 E238 F239 D240 P241 I242 Y243 P244 S245 Y246 T247 A248 L249 Y250 K251 R252 R256 S257 F258 I259 R260 F261 I262 N263 R267 P268 T269 V270 E271 Y272 V273 P274 D275 G276 R277 S280 E281 G282 D283 Y284 L285 L286 T287 Q288 W292 N293 L294 K295
D296 V297 R298 K299 R300 K301 L302 G303 P304 G305 H306 V309 A314 A315 N316 R317 S321 M326 T327 D328 P329 S330 E331 N332 A333 G334 R335 I336 G337 I338 K339 D340 R341 V342 P343 V344 I348 N349 Y354 F355 Y356 Q357 V358 Q361 Y362 K363 I364 V365 V369 R370 H371 S372
G373 G374 G375 K376 PRO GLY ARG D380 C381 S382 P383 R384 V385 N386 I387 V388 R393 K394 R395 D399 P400 A401 T402 C403 T404 S407 D408 L409 L410 S414 V415 E416 I417 P418 V419 V423 T424 P425 V426 V427 D430 S431 R434 K435 T436 L437 S438 T439 G442 S443 W444 K445
A446 Y447 A448 D449 N450 T451 F452 D453 T454 A455 P456 W457 V458 P459 S460 G461 L462 PHE ALA ASP ASP GLU SER THR PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.51Å 63.79Å 114.13Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	71.43 – 3.00 71.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (71.43-3.00) 94.2 (71.51-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0068	Depositor
R, R_{free}	0.192 , 0.282 0.189 , 0.277	Depositor DCC
R_{free} test set	1235 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7009	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.93	3/3622 (0.1%)	0.99	8/4912 (0.2%)
1	B	0.92	3/3526 (0.1%)	1.00	4/4780 (0.1%)
All	All	0.92	6/7148 (0.1%)	1.00	12/9692 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	CYS	CB-SG	-6.57	1.71	1.82
1	A	165	CYS	CB-SG	-6.45	1.71	1.82
1	B	27	GLU	CB-CG	5.44	1.62	1.52
1	A	178	CYS	CB-SG	-5.33	1.73	1.81
1	B	457	TRP	CB-CG	-5.12	1.41	1.50
1	A	246	TYR	CD1-CE1	-5.04	1.31	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	84	LEU	CB-CG-CD1	-6.92	99.24	111.00
1	B	128	SER	N-CA-CB	-6.48	100.78	110.50
1	A	7	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	381	CYS	N-CA-C	6.19	127.72	111.00
1	A	45	ARG	NE-CZ-NH1	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	156	GLY	N-CA-C	5.58	127.05	113.10
1	A	96	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	35	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	233	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	99	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	128	SER	N-CA-CB	-5.03	102.96	110.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	GLY	Peptide
1	A	41	MET	Peptide
1	B	293	ASN	Peptide
1	B	294	LEU	Peptide
1	B	380	ASP	Peptide
1	B	41	MET	Peptide
1	B	8	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3539	0	3493	257	0
1	B	3446	0	3413	260	0
2	A	10	0	0	1	0
2	B	14	0	0	3	0
All	All	7009	0	6906	511	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 37.

All (511) 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:301:LYS:HE2	1:A:301:LYS:C	1.37	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:O	1:A:295:LYS:CD	1.71	1.36
1:A:294:LEU:O	1:A:295:LYS:HD3	1.19	1.35
1:A:300:ARG:NH1	1:A:302:LEU:HD13	1.42	1.31
1:B:131:LYS:O	1:B:135:THR:HG22	1.32	1.26
1:B:271:GLU:OE1	1:B:298:ARG:NH1	1.70	1.24
1:A:301:LYS:C	1:A:301:LYS:CE	2.08	1.20
1:A:301:LYS:CE	1:A:301:LYS:O	1.90	1.19
1:A:278:LEU:CA	1:A:301:LYS:HB2	1.74	1.17
1:A:128:SER:HB3	1:A:131:LYS:HG3	1.15	1.15
1:B:95:THR:HG23	1:B:98:GLN:CD	1.66	1.15
1:A:37:ARG:HB3	1:A:38:PRO:HD2	1.30	1.13
1:B:382:SER:HB2	1:B:383:PRO:HD3	1.18	1.13
1:B:434:ARG:HG2	1:B:434:ARG:HH11	0.96	1.12
1:A:295:LYS:O	1:A:296:ASP:HB3	1.49	1.11
1:A:300:ARG:NH1	1:A:302:LEU:CD1	2.14	1.11
1:A:301:LYS:O	1:A:301:LYS:HE3	1.47	1.09
1:A:128:SER:HB3	1:A:131:LYS:CG	1.82	1.08
1:B:387:ILE:HD11	1:B:424:THR:HB	1.26	1.07
1:B:271:GLU:CD	1:B:298:ARG:HH12	1.59	1.06
1:A:142:LYS:HD2	1:A:142:LYS:H	1.16	1.05
1:B:95:THR:HG23	1:B:98:GLN:OE1	1.56	1.04
1:A:302:LEU:O	1:A:304:PRO:HD2	1.58	1.04
1:B:249:LEU:HA	1:B:257:SER:OG	1.58	1.04
1:B:113:GLN:HB2	1:B:116:ASN:ND2	1.74	1.02
1:B:302:LEU:C	1:B:304:PRO:HD3	1.79	1.02
1:A:278:LEU:CB	1:A:301:LYS:HB2	1.91	1.01
1:A:300:ARG:HH11	1:A:302:LEU:CD2	1.74	1.00
1:A:45:ARG:HH11	1:A:45:ARG:CG	1.71	1.00
1:B:387:ILE:CD1	1:B:424:THR:HB	1.92	0.99
1:A:300:ARG:HH11	1:A:302:LEU:HD22	1.22	0.99
1:A:274:PRO:HG2	1:A:277:ARG:HG3	1.42	0.99
1:B:434:ARG:HG2	1:B:434:ARG:NH1	1.62	0.98
1:A:37:ARG:HB3	1:A:38:PRO:CD	1.93	0.98
1:B:9:ASP:OD2	1:B:10:PRO:HD2	1.62	0.98
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.28	0.97
1:B:156:GLY:HA2	1:B:160:ALA:CB	1.94	0.96
1:A:300:ARG:CZ	1:A:302:LEU:HD13	1.95	0.96
1:B:63:THR:O	1:B:67:ASP:OD2	1.85	0.94
1:B:382:SER:HB2	1:B:383:PRO:CD	1.96	0.94
1:A:395:ARG:HG2	1:A:417:ILE:HD13	1.49	0.94
1:B:453:ASP:O	1:B:454:THR:HG22	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:HG2	1:A:176:LEU:CD2	1.99	0.93
1:B:380:ASP:OD2	1:B:381:CYS:HB2	1.70	0.92
1:B:382:SER:CB	1:B:383:PRO:HD3	2.00	0.92
1:A:278:LEU:HB2	1:A:301:LYS:HB2	1.49	0.91
1:A:321:SER:HB2	1:A:423:VAL:O	1.70	0.91
1:A:100:THR:HG21	1:A:371:HIS:HB2	1.54	0.90
1:B:156:GLY:HA2	1:B:160:ALA:HB2	1.52	0.89
1:B:271:GLU:CD	1:B:298:ARG:NH1	2.20	0.89
1:B:434:ARG:HH11	1:B:434:ARG:CG	1.83	0.89
1:B:131:LYS:O	1:B:135:THR:CG2	2.19	0.89
1:B:128:SER:HB3	1:B:131:LYS:HG3	1.55	0.89
1:B:95:THR:CG2	1:B:98:GLN:CD	2.41	0.88
1:A:278:LEU:HA	1:A:301:LYS:HB2	1.54	0.88
1:B:416:GLU:N	1:B:416:GLU:OE1	2.05	0.88
1:B:277:ARG:NH2	1:B:300:ARG:HD2	1.88	0.88
1:A:458:VAL:HG13	1:A:459:PRO:HD2	1.53	0.87
1:A:376:LYS:HB2	1:A:379:ARG:HH22	1.39	0.87
1:B:303:GLY:N	1:B:304:PRO:HD3	1.86	0.87
1:A:301:LYS:HE2	1:A:302:LEU:N	1.90	0.87
1:A:170:LYS:HB2	1:A:185:ARG:HH11	1.40	0.86
1:A:294:LEU:O	1:A:295:LYS:CG	2.23	0.86
1:B:277:ARG:HH21	1:B:300:ARG:HD2	1.40	0.86
1:B:327:THR:CG2	1:B:339:LYS:HB2	2.04	0.86
1:B:387:ILE:HD11	1:B:424:THR:CB	2.05	0.86
1:A:465:ASP:HB2	1:B:252:ARG:NH2	1.91	0.85
1:A:45:ARG:HG2	1:A:45:ARG:NH1	1.88	0.84
1:B:114:SER:O	1:B:115:GLU:HB2	1.77	0.84
1:A:113:GLN:HB2	1:A:116:ASN:HB2	1.60	0.84
1:A:457:TRP:HE3	1:A:458:VAL:H	1.25	0.83
1:B:206:VAL:O	1:B:207:ASN:HB2	1.75	0.83
1:B:286:LEU:HD11	1:B:349:ASN:HA	1.60	0.83
1:B:370:ARG:HD3	1:B:376:LYS:HD3	1.61	0.83
1:A:293:ASN:C	1:A:294:LEU:HD23	1.99	0.82
1:A:200:VAL:HG12	1:A:201:SER:N	1.93	0.81
1:B:127:ILE:HG23	1:B:135:THR:HG21	1.60	0.81
1:B:113:GLN:CB	1:B:116:ASN:ND2	2.43	0.81
1:B:116:ASN:H	1:B:116:ASN:HD22	1.29	0.80
1:A:395:ARG:HG2	1:A:417:ILE:CD1	2.11	0.80
1:A:142:LYS:H	1:A:142:LYS:CD	1.95	0.79
1:B:141:THR:O	1:B:145:GLU:HG2	1.83	0.78
1:A:45:ARG:HH11	1:A:45:ARG:CB	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LYS:HE2	1:A:301:LYS:CA	2.12	0.78
1:B:382:SER:CB	1:B:383:PRO:CD	2.57	0.78
1:B:380:ASP:CG	1:B:381:CYS:N	2.36	0.77
1:B:97:GLU:O	1:B:101:VAL:HG23	1.83	0.77
1:A:45:ARG:NH1	1:A:196:GLY:O	2.16	0.77
1:A:460:SER:O	1:A:462:LEU:N	2.16	0.77
1:A:170:LYS:CB	1:A:185:ARG:HH11	1.96	0.77
1:B:40:GLN:HB2	1:B:88:TYR:OH	1.84	0.77
1:A:293:ASN:O	1:A:294:LEU:HD23	1.84	0.77
1:B:376:LYS:HA	1:B:380:ASP:OD2	1.85	0.77
1:A:465:ASP:HB2	1:B:252:ARG:HH21	1.47	0.77
1:B:327:THR:HG22	1:B:339:LYS:HB2	1.66	0.76
1:B:8:GLU:OE1	1:B:8:GLU:N	2.18	0.76
1:A:294:LEU:O	1:A:295:LYS:CB	2.34	0.76
1:B:156:GLY:HA2	1:B:160:ALA:HB3	1.66	0.76
1:B:258:PHE:CZ	1:B:262:ILE:HD12	2.20	0.76
1:B:219:ASP:HB3	1:B:381:CYS:O	1.85	0.76
1:B:453:ASP:O	1:B:454:THR:CG2	2.34	0.76
1:A:129:SER:HB3	1:A:360:LEU:HD23	1.66	0.76
1:B:61:GLY:O	1:B:63:THR:HG23	1.86	0.76
1:A:384:ARG:NH1	1:A:384:ARG:HG2	2.00	0.75
1:A:142:LYS:HD2	1:A:142:LYS:N	1.97	0.75
1:A:384:ARG:HG2	1:A:384:ARG:HH11	1.51	0.75
1:A:175:LYS:HG2	1:A:176:LEU:HD23	1.67	0.75
1:A:277:ARG:C	1:A:301:LYS:HB3	2.07	0.75
1:B:72:LEU:HD12	1:B:72:LEU:N	2.02	0.75
1:A:358:VAL:HG13	1:A:385:VAL:HG11	1.69	0.74
1:B:271:GLU:OE1	1:B:280:SER:HB3	1.86	0.74
1:A:295:LYS:O	1:A:296:ASP:CB	2.29	0.73
1:B:25:SER:HB3	1:B:27:GLU:OE1	1.87	0.73
1:A:460:SER:C	1:A:462:LEU:H	1.91	0.73
1:B:200:VAL:HG21	1:B:361:GLN:HG2	1.71	0.73
1:B:339:LYS:HG2	1:B:340:ASP:OD2	1.89	0.72
1:B:164:ARG:NH2	1:B:416:GLU:OE2	2.18	0.72
1:A:96:ASP:O	1:A:100:THR:HG22	1.90	0.72
1:A:278:LEU:HB2	1:A:301:LYS:CB	2.19	0.72
1:A:435:LYS:O	1:A:439:THR:HG23	1.91	0.71
1:B:434:ARG:NH1	1:B:434:ARG:CG	2.43	0.71
1:B:302:LEU:C	1:B:304:PRO:CD	2.58	0.70
1:A:300:ARG:HH11	1:A:302:LEU:CG	2.04	0.70
1:B:272:TYR:CE1	1:B:293:ASN:ND2	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:N	1:A:301:LYS:HB2	2.06	0.70
1:A:294:LEU:O	1:A:295:LYS:HD2	1.87	0.69
1:B:89:TRP:CZ2	2:B:2002:HOH:O	2.44	0.69
1:A:302:LEU:O	1:A:304:PRO:CD	2.39	0.69
1:A:45:ARG:HH11	1:A:45:ARG:HB2	1.55	0.69
1:A:300:ARG:NE	1:A:302:LEU:HB2	2.07	0.69
1:A:202:LEU:HD23	1:A:361:GLN:HG2	1.74	0.69
1:A:300:ARG:HE	1:A:302:LEU:HB2	1.58	0.68
1:B:46:PHE:HB2	1:B:91:LEU:HD13	1.75	0.68
1:A:68:PHE:HD2	1:A:102:LEU:HD21	1.59	0.68
1:A:96:ASP:O	1:A:100:THR:CG2	2.41	0.68
1:A:113:GLN:HG3	1:A:116:ASN:HB2	1.76	0.68
1:A:200:VAL:HG12	1:A:201:SER:O	1.93	0.68
1:B:95:THR:CG2	1:B:98:GLN:OE1	2.39	0.67
1:B:302:LEU:O	1:B:304:PRO:CD	2.42	0.67
1:B:301:LYS:O	1:B:304:PRO:CD	2.42	0.67
1:A:379:ARG:CB	1:A:379:ARG:HH21	2.07	0.67
1:A:294:LEU:C	1:A:295:LYS:HD3	2.12	0.67
1:A:158:PRO:O	1:A:161:PHE:HB3	1.96	0.66
1:A:376:LYS:HB2	1:A:379:ARG:NH2	2.10	0.66
1:A:460:SER:C	1:A:462:LEU:N	2.48	0.66
1:A:278:LEU:CA	1:A:301:LYS:CB	2.64	0.66
1:A:379:ARG:HH21	1:A:379:ARG:HB2	1.59	0.66
1:A:170:LYS:HB2	1:A:185:ARG:NH1	2.10	0.66
1:B:89:TRP:CH2	2:B:2002:HOH:O	2.48	0.66
1:B:453:ASP:O	1:B:454:THR:CB	2.41	0.66
1:A:38:PRO:HG2	1:A:457:TRP:HD1	1.58	0.65
1:A:57:GLN:NE2	1:A:63:THR:HA	2.12	0.65
1:A:113:GLN:CB	1:A:116:ASN:HB2	2.25	0.65
1:B:275:ASP:CG	1:B:317:ARG:HH12	1.99	0.65
1:B:453:ASP:C	1:B:454:THR:HG22	2.16	0.65
1:B:113:GLN:HB2	1:B:116:ASN:HD21	1.61	0.65
1:A:200:VAL:CG1	1:A:201:SER:N	2.61	0.64
1:B:277:ARG:HH21	1:B:300:ARG:CD	2.09	0.64
1:A:175:LYS:HG2	1:A:176:LEU:HD21	1.76	0.64
1:A:272:TYR:CE1	1:A:274:PRO:HD3	2.32	0.64
1:A:296:ASP:CG	1:A:297:VAL:N	2.51	0.64
1:A:170:LYS:CB	1:A:185:ARG:NH1	2.59	0.64
1:A:454:THR:O	1:A:455:ALA:C	2.36	0.64
1:A:300:ARG:NH1	1:A:302:LEU:HD22	2.05	0.64
1:A:169:VAL:HG11	1:A:226:ILE:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ASP:OD2	1:A:414:SER:OG	2.16	0.63
1:A:140:PRO:HG2	1:A:447:TYR:HB2	1.80	0.63
1:B:95:THR:HG23	1:B:98:GLN:CG	2.29	0.63
1:A:82:PRO:HG2	1:A:87:ILE:CD1	2.29	0.63
1:A:301:LYS:CE	1:A:302:LEU:N	2.57	0.63
1:B:404:THR:HG22	1:B:410:LEU:HA	1.80	0.63
1:A:40:GLN:HB2	1:A:92:GLN:NE2	2.14	0.63
1:B:29:GLU:OE1	1:B:33:ARG:NH1	2.30	0.63
1:A:278:LEU:N	1:A:301:LYS:CB	2.61	0.62
1:A:278:LEU:HD13	1:A:306:HIS:CE1	2.34	0.62
1:A:465:ASP:CB	1:B:252:ARG:NH2	2.61	0.62
1:A:464:ALA:O	1:A:465:ASP:HB2	1.98	0.62
1:B:462:LEU:C	1:B:462:LEU:HD22	2.19	0.62
1:A:229:ARG:NH2	1:A:283:ASP:OD1	2.32	0.62
1:B:327:THR:CG2	1:B:339:LYS:CB	2.78	0.62
1:B:41:MET:HB2	1:B:456:PRO:HB2	1.81	0.62
1:B:72:LEU:N	1:B:72:LEU:CD1	2.62	0.62
1:B:327:THR:HG23	1:B:339:LYS:HB2	1.81	0.62
1:B:399:ASP:O	1:B:400:PRO:C	2.38	0.62
1:B:462:LEU:C	1:B:462:LEU:CD2	2.67	0.62
1:B:400:PRO:O	1:B:402:THR:N	2.31	0.61
1:A:321:SER:CB	1:A:423:VAL:O	2.47	0.61
1:B:304:PRO:O	1:B:305:GLY:C	2.37	0.61
1:B:57:GLN:C	1:B:59:PHE:H	2.01	0.61
1:B:380:ASP:OD2	1:B:381:CYS:CB	2.46	0.61
1:B:140:PRO:HD3	1:B:443:SER:HB2	1.81	0.61
1:B:110:THR:O	1:B:119:TRP:CZ3	2.54	0.61
1:B:430:ASP:O	1:B:434:ARG:HB2	2.01	0.61
1:B:107:GLU:OE1	1:B:111:ARG:HG3	2.00	0.61
1:B:249:LEU:HA	1:B:257:SER:HG	1.64	0.61
1:A:113:GLN:CG	1:A:116:ASN:HB2	2.31	0.60
1:B:169:VAL:HA	1:B:172:ILE:HD12	1.83	0.60
1:A:280:SER:OG	1:A:281:GLU:N	2.32	0.60
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.02	0.60
1:A:362:TYR:CG	1:A:428:LEU:HD12	2.37	0.60
1:A:387:ILE:HG22	1:A:424:THR:HB	1.84	0.60
1:A:34:ASN:N	1:A:34:ASN:OD1	2.35	0.60
1:A:303:GLY:HA3	1:A:306:HIS:HB2	1.83	0.59
1:B:68:PHE:O	1:B:72:LEU:CD1	2.50	0.59
1:B:246:TYR:O	1:B:249:LEU:HB3	2.02	0.59
1:A:278:LEU:HA	1:A:301:LYS:CB	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LYS:HA	1:A:243:TYR:CD2	2.37	0.59
1:A:100:THR:HG21	1:A:371:HIS:CB	2.31	0.59
1:B:301:LYS:O	1:B:304:PRO:CG	2.50	0.59
1:B:327:THR:HG23	1:B:339:LYS:CB	2.33	0.59
1:A:82:PRO:HG2	1:A:87:ILE:HD12	1.83	0.58
1:A:301:LYS:O	1:A:301:LYS:CG	2.51	0.58
1:B:229:ARG:NH2	1:B:269:THR:OG1	2.36	0.58
1:A:458:VAL:HG13	1:A:459:PRO:CD	2.31	0.58
1:B:321:SER:HB3	1:B:423:VAL:O	2.03	0.58
1:B:370:ARG:O	1:B:374:GLY:HA2	2.03	0.58
1:A:31:PHE:CE2	1:A:35:LEU:HD23	2.37	0.58
1:A:306:HIS:O	1:A:308:LEU:N	2.37	0.58
1:B:57:GLN:O	1:B:59:PHE:N	2.37	0.58
1:B:443:SER:HA	1:B:446:ALA:HB3	1.83	0.58
1:A:362:TYR:HB2	1:A:385:VAL:HG21	1.86	0.58
1:B:343:PRO:O	1:B:344:VAL:HG13	2.04	0.58
1:A:286:LEU:HG	1:A:349:ASN:HB2	1.84	0.57
1:B:286:LEU:CD1	1:B:349:ASN:HA	2.31	0.57
1:B:246:TYR:CE1	1:B:419:VAL:HG13	2.40	0.57
1:B:386:ASN:HD22	1:B:425:PRO:HA	1.69	0.57
1:A:200:VAL:HG23	1:A:364:ILE:HD12	1.86	0.57
1:B:227:LYS:HE3	1:B:354:TYR:CD1	2.40	0.57
1:B:302:LEU:O	1:B:304:PRO:HD2	2.05	0.57
1:A:38:PRO:CG	1:A:457:TRP:HD1	2.18	0.57
1:A:236:LYS:HB3	1:A:243:TYR:CZ	2.40	0.57
1:B:9:ASP:OD2	1:B:10:PRO:CD	2.47	0.57
1:A:223:ILE:HD12	1:A:385:VAL:HG22	1.86	0.56
1:B:240:ASP:OD1	1:B:243:TYR:N	2.37	0.56
1:A:291:ALA:C	1:A:293:ASN:H	2.09	0.56
1:B:73:VAL:HG13	1:B:90:GLY:HA3	1.86	0.56
1:A:287:THR:HG21	1:A:292:TRP:CG	2.41	0.56
1:A:87:ILE:HG23	1:A:91:LEU:HD12	1.87	0.56
1:B:10:PRO:HG2	1:B:59:PHE:CE2	2.41	0.56
1:B:415:VAL:HG12	1:B:416:GLU:O	2.06	0.55
1:B:304:PRO:HD2	1:B:306:HIS:HB2	1.88	0.55
1:A:178:CYS:O	1:A:179:GLY:C	2.43	0.55
1:A:294:LEU:O	1:A:295:LYS:HB3	2.05	0.55
1:A:38:PRO:HG2	1:A:457:TRP:CD1	2.39	0.55
1:A:301:LYS:NZ	1:A:302:LEU:HD12	2.21	0.55
1:A:301:LYS:O	1:A:301:LYS:CD	2.54	0.55
1:B:182:SER:O	1:B:183:ALA:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:CD2	1:A:361:GLN:HG2	2.37	0.55
1:A:328:ASP:OD1	1:A:330:SER:HB2	2.06	0.55
1:B:387:ILE:CG1	1:B:424:THR:HB	2.37	0.55
1:B:430:ASP:O	1:B:431:SER:C	2.44	0.55
1:B:180:ASP:OD1	1:B:180:ASP:N	2.27	0.55
1:B:369:VAL:O	1:B:370:ARG:C	2.45	0.55
1:A:93:GLU:OE2	1:B:335:ARG:HD3	2.07	0.54
1:A:128:SER:HB3	1:A:131:LYS:CD	2.37	0.54
1:A:277:ARG:C	1:A:301:LYS:CB	2.76	0.54
1:A:278:LEU:HB2	1:A:301:LYS:CA	2.36	0.54
1:B:106:VAL:O	1:B:109:MET:HB3	2.07	0.54
1:B:10:PRO:HG2	1:B:59:PHE:HE2	1.71	0.54
1:B:287:THR:HG21	1:B:292:TRP:CD1	2.42	0.54
1:B:175:LYS:HG3	1:B:181:ALA:HB2	1.90	0.54
1:A:83:SER:O	1:A:84:LEU:C	2.45	0.54
1:B:41:MET:HE3	1:B:41:MET:HA	1.89	0.54
1:A:301:LYS:HZ3	1:A:302:LEU:HD12	1.73	0.54
1:A:359:LEU:O	1:A:362:TYR:HB3	2.08	0.54
1:A:277:ARG:HA	1:A:301:LYS:H	1.73	0.54
1:A:328:ASP:C	1:A:330:SER:H	2.10	0.54
1:B:238:GLU:HB2	2:B:2009:HOH:O	2.08	0.54
1:A:460:SER:HA	1:A:463:PHE:CD2	2.43	0.53
1:A:25:SER:O	1:A:26:PRO:C	2.47	0.53
1:A:40:GLN:CB	1:A:92:GLN:NE2	2.71	0.53
1:A:300:ARG:NH1	1:A:302:LEU:CG	2.66	0.53
1:B:380:ASP:CG	1:B:381:CYS:H	2.12	0.53
1:A:170:LYS:HB3	1:A:185:ARG:NH1	2.22	0.53
1:A:364:ILE:O	1:A:367:ASP:HB2	2.08	0.53
1:B:56:ILE:HA	1:B:59:PHE:CE1	2.43	0.53
1:B:110:THR:O	1:B:119:TRP:HZ3	1.91	0.53
1:B:132:LEU:O	1:B:135:THR:HG23	2.09	0.53
1:B:395:ARG:HG2	1:B:417:ILE:HD12	1.91	0.53
1:B:41:MET:O	1:B:459:PRO:HD3	2.08	0.53
1:B:234:PHE:HB3	1:B:242:ILE:HD12	1.89	0.53
1:B:400:PRO:C	1:B:402:THR:N	2.61	0.53
1:A:300:ARG:NH1	1:A:302:LEU:CD2	2.58	0.52
1:B:16:SER:O	1:B:21:ARG:HD3	2.08	0.52
1:B:107:GLU:OE1	1:B:188:GLY:N	2.39	0.52
1:B:40:GLN:OE1	1:B:40:GLN:HA	2.09	0.52
1:A:89:TRP:CE3	1:A:89:TRP:HA	2.44	0.52
1:A:173:VAL:HA	1:A:177:ILE:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:HD12	1:A:412:ASP:N	2.24	0.52
1:B:72:LEU:CD1	1:B:72:LEU:H	2.22	0.52
1:B:277:ARG:HD3	1:B:298:ARG:O	2.09	0.52
1:B:330:SER:HB3	1:B:399:ASP:OD1	2.09	0.52
1:A:300:ARG:HH11	1:A:302:LEU:CD1	2.03	0.52
1:A:438:SER:HB3	1:A:464:ALA:HB2	1.90	0.52
1:B:68:PHE:O	1:B:72:LEU:HD13	2.10	0.52
1:B:105:TYR:O	1:B:109:MET:HB2	2.08	0.52
1:B:272:TYR:CZ	1:B:293:ASN:ND2	2.77	0.52
1:B:107:GLU:OE2	1:B:111:ARG:NH2	2.42	0.52
1:A:114:SER:HA	1:A:119:TRP:CE3	2.45	0.52
1:B:57:GLN:C	1:B:59:PHE:N	2.62	0.52
1:A:249:LEU:HA	1:A:257:SER:OG	2.09	0.52
1:B:453:ASP:O	1:B:454:THR:HB	2.07	0.52
1:A:31:PHE:HE2	1:A:35:LEU:HD23	1.75	0.52
1:A:301:LYS:O	1:A:301:LYS:HG2	2.10	0.52
1:B:386:ASN:ND2	1:B:425:PRO:HA	2.25	0.52
1:B:246:TYR:CE1	1:B:419:VAL:CG1	2.93	0.52
1:B:326:MET:CE	1:B:338:ILE:HD12	2.40	0.52
1:A:207:ASN:HB2	1:A:220:ARG:O	2.10	0.51
1:B:443:SER:O	1:B:444:TRP:C	2.47	0.51
1:A:412:ASP:OD2	1:A:414:SER:N	2.35	0.51
1:B:240:ASP:HB3	1:B:243:TYR:HB3	1.91	0.51
1:B:43:ALA:O	1:B:47:VAL:HG23	2.10	0.51
1:A:278:LEU:HB2	1:A:301:LYS:HA	1.92	0.51
1:B:140:PRO:HG2	1:B:447:TYR:CB	2.40	0.51
1:B:293:ASN:O	1:B:294:LEU:HG	2.11	0.51
1:A:411:LEU:HD12	1:A:412:ASP:H	1.74	0.51
1:B:192:SER:HB2	1:B:364:ILE:HG12	1.91	0.51
1:A:47:VAL:O	1:A:50:TYR:HB3	2.11	0.51
1:B:19:PHE:CG	1:B:45:ARG:NH1	2.78	0.51
1:B:355:PHE:O	1:B:358:VAL:HG12	2.10	0.51
1:A:306:HIS:O	1:A:307:ASP:C	2.49	0.50
1:B:256:ARG:HG2	1:B:260:ARG:HH21	1.75	0.50
1:B:273:VAL:HG11	1:B:286:LEU:HD22	1.93	0.50
1:B:445:LYS:HE2	1:B:456:PRO:O	2.11	0.50
1:A:45:ARG:NH1	1:A:45:ARG:HB2	2.24	0.50
1:B:206:VAL:O	1:B:207:ASN:CB	2.48	0.50
1:B:400:PRO:HG2	1:B:403:CYS:SG	2.51	0.50
1:B:59:PHE:O	1:B:59:PHE:CD2	2.64	0.50
1:A:200:VAL:CG1	1:A:201:SER:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:THR:HA	1:B:283:ASP:OD2	2.12	0.50
1:A:46:PHE:HB3	1:A:91:LEU:HD22	1.93	0.49
1:B:8:GLU:N	1:B:8:GLU:CD	2.66	0.49
1:B:47:VAL:HG22	1:B:91:LEU:HD12	1.94	0.49
1:B:69:VAL:O	1:B:72:LEU:HD13	2.12	0.49
1:B:338:ILE:N	1:B:338:ILE:HD13	2.28	0.49
1:A:129:SER:CB	1:A:360:LEU:HD23	2.41	0.49
1:A:272:TYR:CD1	1:A:274:PRO:HD3	2.48	0.49
1:B:14:MET:HE1	1:B:55:GLN:HB2	1.95	0.49
1:A:362:TYR:OH	1:A:382:SER:HB3	2.13	0.49
1:B:284:TYR:O	1:B:348:ILE:HD12	2.13	0.49
1:B:451:THR:O	1:B:451:THR:CG2	2.59	0.49
1:A:273:VAL:HG11	1:A:286:LEU:HD22	1.94	0.49
1:A:393:ARG:NH2	1:A:399:ASP:OD1	2.46	0.48
1:B:114:SER:O	1:B:115:GLU:CB	2.54	0.48
1:A:384:ARG:HH11	1:A:384:ARG:CG	2.15	0.48
1:A:119:TRP:O	1:A:123:ARG:HG3	2.13	0.48
1:A:277:ARG:HD2	1:A:298:ARG:O	2.14	0.48
1:B:295:LYS:O	1:B:296:ASP:OD1	2.31	0.48
1:A:207:ASN:CB	1:A:220:ARG:O	2.62	0.48
1:A:421:VAL:HG12	1:A:421:VAL:O	2.13	0.48
1:B:299:LYS:C	1:B:300:ARG:O	2.51	0.48
1:B:303:GLY:N	1:B:304:PRO:CD	2.68	0.48
1:A:308:LEU:HD23	1:A:308:LEU:C	2.33	0.48
1:B:127:ILE:CG2	1:B:135:THR:HG21	2.35	0.48
1:B:258:PHE:CZ	1:B:262:ILE:CD1	2.93	0.48
1:B:40:GLN:CB	1:B:88:TYR:OH	2.58	0.48
1:A:31:PHE:CD2	1:A:31:PHE:C	2.87	0.48
1:A:68:PHE:HD2	1:A:102:LEU:CD2	2.26	0.48
1:A:441:ALA:O	1:A:444:TRP:HB3	2.13	0.48
1:B:200:VAL:CG2	1:B:361:GLN:HG2	2.43	0.48
1:B:197:ILE:HG22	1:B:198:PHE:CG	2.49	0.48
1:A:192:SER:OG	1:A:195:ASP:OD1	2.30	0.48
1:B:41:MET:SD	1:B:44:MET:HB2	2.53	0.48
1:A:83:SER:O	1:A:85:LYS:N	2.47	0.47
1:A:173:VAL:HA	1:A:177:ILE:HG13	1.95	0.47
1:B:234:PHE:HB2	1:B:240:ASP:OD2	2.14	0.47
1:B:180:ASP:C	1:B:182:SER:H	2.17	0.47
1:B:113:GLN:CB	1:B:116:ASN:CG	2.83	0.47
1:B:365:VAL:O	1:B:369:VAL:HG23	2.14	0.47
1:A:96:ASP:O	1:A:100:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:HE3	1:A:354:TYR:CE1	2.50	0.47
1:A:53:CYS:O	1:A:54:LYS:C	2.53	0.47
1:B:161:PHE:CZ	1:B:233:LEU:HD13	2.49	0.47
1:B:258:PHE:CE1	1:B:262:ILE:HD12	2.50	0.47
1:A:175:LYS:CG	1:A:176:LEU:HD23	2.41	0.47
1:B:259:ILE:O	1:B:263:ASN:HB2	2.14	0.47
1:B:326:MET:HE1	1:B:338:ILE:HD12	1.97	0.47
1:B:404:THR:HG22	1:B:410:LEU:CA	2.45	0.47
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.60	0.47
1:A:140:PRO:HG2	1:A:447:TYR:CB	2.43	0.47
1:B:172:ILE:HG23	1:B:176:LEU:HD12	1.97	0.46
1:B:301:LYS:O	1:B:304:PRO:HG2	2.15	0.46
1:A:287:THR:HG21	1:A:292:TRP:CB	2.46	0.46
1:B:251:LYS:HE3	1:B:251:LYS:HB3	1.85	0.46
1:A:45:ARG:CG	1:A:45:ARG:NH1	2.43	0.46
1:A:219:ASP:HB2	1:A:381:CYS:HB3	1.98	0.46
1:B:41:MET:HA	1:B:41:MET:CE	2.46	0.46
1:B:301:LYS:O	1:B:304:PRO:HD3	2.14	0.46
1:B:302:LEU:HB3	1:B:303:GLY:H	1.47	0.46
1:B:316:ASN:OD1	1:B:427:VAL:N	2.43	0.46
1:A:328:ASP:O	1:A:330:SER:N	2.48	0.46
1:A:116:ASN:OD1	1:A:117:LEU:N	2.48	0.46
1:A:296:ASP:OD2	1:A:297:VAL:O	2.34	0.46
1:A:306:HIS:C	1:A:308:LEU:N	2.67	0.46
1:A:387:ILE:CG2	1:A:424:THR:HB	2.46	0.46
1:B:73:VAL:CG1	1:B:90:GLY:HA3	2.46	0.46
1:B:100:THR:HG21	1:B:371:HIS:HB2	1.98	0.46
1:B:327:THR:HG22	1:B:339:LYS:CB	2.41	0.46
1:A:82:PRO:HB2	1:A:86:SER:HB2	1.98	0.46
1:A:276:GLY:HA2	1:A:301:LYS:HZ3	1.81	0.46
1:A:365:VAL:HA	1:A:368:TYR:HD1	1.81	0.46
1:A:435:LYS:HD3	1:A:439:THR:CG2	2.45	0.46
1:A:238:GLU:HG2	1:A:239:PHE:CE2	2.51	0.45
1:A:112:GLY:O	1:A:113:GLN:C	2.55	0.45
1:A:291:ALA:C	1:A:293:ASN:N	2.70	0.45
1:B:295:LYS:HB3	1:B:296:ASP:H	1.50	0.45
1:A:261:PHE:O	1:A:262:ILE:C	2.52	0.45
1:A:399:ASP:HA	1:A:400:PRO:HD2	1.79	0.45
1:A:460:SER:HA	1:A:463:PHE:CG	2.52	0.45
1:B:226:ILE:O	1:B:227:LYS:HD2	2.17	0.45
1:A:400:PRO:O	1:A:401:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLN:O	1:B:361:GLN:HG3	2.17	0.45
1:B:404:THR:HB	1:B:409:LEU:H	1.82	0.45
1:A:30:ALA:O	1:A:33:ARG:N	2.48	0.45
1:B:40:GLN:N	1:B:88:TYR:OH	2.47	0.45
1:A:29:GLU:O	1:A:30:ALA:C	2.54	0.45
1:B:133:LEU:HD22	1:B:356:TYR:CD1	2.52	0.44
1:B:197:ILE:HG21	1:B:197:ILE:HD13	1.69	0.44
1:A:250:TYR:HE2	1:A:326:MET:O	2.01	0.44
1:A:379:ARG:NH2	1:A:379:ARG:HB2	2.27	0.44
1:A:73:VAL:O	1:A:74:GLN:C	2.55	0.44
1:A:140:PRO:O	1:A:141:THR:C	2.53	0.44
1:A:273:VAL:HA	1:A:274:PRO:HD2	1.67	0.44
1:B:47:VAL:O	1:B:48:TYR:C	2.55	0.44
1:B:316:ASN:OD1	1:B:427:VAL:HB	2.18	0.44
1:B:174:CYS:SG	1:B:183:ALA:HB3	2.57	0.44
1:B:435:LYS:O	1:B:439:THR:CG2	2.66	0.44
1:A:65:PHE:CE1	1:A:102:LEU:HB3	2.52	0.44
1:B:273:VAL:HA	1:B:274:PRO:HD3	1.81	0.44
1:A:46:PHE:CB	1:A:91:LEU:HD22	2.47	0.44
1:A:68:PHE:CD2	1:A:102:LEU:HD21	2.47	0.44
1:A:183:ALA:HB1	1:A:205:CYS:O	2.18	0.44
1:A:112:GLY:C	1:A:113:GLN:HG2	2.37	0.44
1:B:256:ARG:CG	1:B:260:ARG:HH21	2.31	0.44
1:B:46:PHE:CB	1:B:91:LEU:HD13	2.47	0.43
1:B:227:LYS:HE3	1:B:354:TYR:CE1	2.53	0.43
1:A:402:THR:HG22	1:A:403:CYS:N	2.32	0.43
1:B:141:THR:C	1:B:143:VAL:H	2.21	0.43
1:B:344:VAL:HG23	1:B:344:VAL:O	2.19	0.43
1:B:243:TYR:N	1:B:244:PRO:CD	2.81	0.43
1:B:227:LYS:N	1:B:388:VAL:O	2.49	0.43
1:A:255:LYS:HE2	2:A:2008:HOH:O	2.19	0.43
1:B:56:ILE:HA	1:B:59:PHE:CD1	2.53	0.43
1:B:61:GLY:O	1:B:63:THR:N	2.52	0.43
1:A:95:THR:HG21	1:B:178:CYS:O	2.19	0.43
1:B:400:PRO:C	1:B:402:THR:H	2.20	0.43
1:A:226:ILE:HG22	1:A:227:LYS:N	2.33	0.43
1:A:113:GLN:HB2	1:A:116:ASN:CB	2.41	0.43
1:B:37:ARG:HB2	1:B:38:PRO:CD	2.49	0.43
1:B:332:ASN:O	1:B:333:ALA:C	2.57	0.43
1:A:37:ARG:CB	1:A:38:PRO:CD	2.74	0.42
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:HG22	1:B:198:PHE:CD2	2.54	0.42
1:B:337:GLY:O	1:B:338:ILE:C	2.54	0.42
1:A:68:PHE:CD2	1:A:102:LEU:CD2	3.02	0.42
1:A:87:ILE:O	1:A:88:TYR:C	2.57	0.42
1:B:335:ARG:NH1	1:B:407:SER:OG	2.52	0.42
1:B:380:ASP:CG	1:B:381:CYS:CB	2.87	0.42
1:B:393:ARG:HG2	1:B:419:VAL:CG2	2.49	0.42
1:A:25:SER:HA	1:A:26:PRO:HD2	1.66	0.42
1:A:429:PRO:HG2	1:A:432:VAL:CG2	2.50	0.42
1:B:249:LEU:HD13	1:B:258:PHE:HA	2.01	0.42
1:B:452:PHE:C	1:B:454:THR:H	2.20	0.42
1:A:184:ASN:ND2	1:A:186:GLN:O	2.50	0.42
1:A:254:CYS:O	1:A:255:LYS:C	2.58	0.42
1:B:11:MET:HE3	1:B:11:MET:HB3	1.82	0.42
1:B:343:PRO:O	1:B:344:VAL:CG1	2.68	0.42
1:B:376:LYS:HE2	1:B:376:LYS:HB2	1.68	0.42
1:B:225:GLU:OE2	1:B:225:GLU:HA	2.20	0.42
1:A:57:GLN:HA	1:A:60:SER:O	2.20	0.42
1:B:240:ASP:O	1:B:244:PRO:HD3	2.20	0.42
1:B:247:THR:O	1:B:248:ALA:C	2.56	0.42
1:B:294:LEU:HA	1:B:294:LEU:HD23	1.51	0.42
1:A:31:PHE:HB3	1:A:84:LEU:HD12	2.01	0.42
1:A:387:ILE:HG22	1:A:387:ILE:O	2.20	0.42
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.77	0.41
1:B:183:ALA:O	1:B:185:ARG:NE	2.44	0.41
1:B:437:LEU:HD23	1:B:437:LEU:HA	1.74	0.41
1:A:133:LEU:HD13	1:A:356:TYR:CE1	2.55	0.41
1:B:375:GLY:O	1:B:380:ASP:HA	2.20	0.41
1:A:119:TRP:CH2	1:A:188:GLY:HA2	2.55	0.41
1:A:229:ARG:NH2	1:A:269:THR:OG1	2.52	0.41
1:B:451:THR:O	1:B:451:THR:HG22	2.19	0.41
1:A:424:THR:HA	1:A:425:PRO:HD2	1.94	0.41
1:B:328:ASP:C	1:B:328:ASP:OD1	2.59	0.41
1:A:324:TYR:CD1	1:A:324:TYR:N	2.88	0.41
1:B:156:GLY:CA	1:B:160:ALA:HB2	2.36	0.41
1:B:229:ARG:HH12	1:B:231:LYS:HE2	1.84	0.41
1:A:294:LEU:C	1:A:295:LYS:CG	2.87	0.41
1:A:405:LEU:HB2	1:A:409:LEU:HD23	2.02	0.41
1:A:447:TYR:O	1:A:448:ALA:C	2.58	0.41
1:A:465:ASP:CB	1:B:252:ARG:HH22	2.33	0.41
1:B:287:THR:HG21	1:B:292:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG12	1:A:416:GLU:O	2.20	0.41
1:B:140:PRO:HG2	1:B:447:TYR:CG	2.56	0.41
1:B:361:GLN:O	1:B:362:TYR:C	2.59	0.41
1:B:445:LYS:NZ	1:B:449:ASP:OD1	2.49	0.41
1:B:280:SER:OG	1:B:281:GLU:N	2.54	0.41
1:A:161:PHE:CG	1:A:230:PHE:HD1	2.39	0.40
1:A:348:ILE:HD12	1:A:348:ILE:HA	1.94	0.40
1:A:412:ASP:HB3	1:A:415:VAL:HG23	2.03	0.40
1:B:197:ILE:HG22	1:B:198:PHE:N	2.37	0.40
1:A:30:ALA:O	1:A:33:ARG:HB3	2.22	0.40
1:A:262:ILE:HG21	1:A:270:VAL:CG2	2.51	0.40
1:A:300:ARG:HG3	1:A:302:LEU:H	1.87	0.40
1:A:41:MET:CB	1:A:457:TRP:O	2.70	0.40
1:A:247:THR:HG22	1:A:251:LYS:HD2	2.03	0.40
1:A:294:LEU:HD23	1:A:294:LEU:N	2.31	0.40
1:B:256:ARG:HG2	1:B:260:ARG:NH2	2.37	0.40
1:B:386:ASN:HD22	1:B:425:PRO:CA	2.34	0.40
1:B:73:VAL:CG1	1:B:90:GLY:CA	3.00	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	443/470 (94%)	364 (82%)	57 (13%)	22 (5%)	2 12
1	B	429/470 (91%)	347 (81%)	59 (14%)	23 (5%)	2 11
All	All	872/940 (93%)	711 (82%)	116 (13%)	45 (5%)	2 12

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	PRO
1	A	295	LYS
1	A	296	ASP
1	A	465	ASP
1	B	42	PRO
1	B	115	GLU
1	B	295	LYS
1	B	454	THR
1	A	84	LEU
1	A	112	GLY
1	A	113	GLN
1	A	244	PRO
1	A	280	SER
1	A	461	GLY
1	B	58	GLU
1	B	62	GLU
1	B	114	SER
1	B	207	ASN
1	B	296	ASP
1	B	302	LEU
1	B	304	PRO
1	B	370	ARG
1	B	401	ALA
1	B	442	GLY
1	A	146	PRO
1	A	245	SER
1	B	314	ALA
1	B	383	PRO
1	B	434	ARG
1	A	26	PRO
1	A	37	ARG
1	B	9	ASP
1	B	373	GLY
1	A	282	GLY
1	A	400	PRO
1	A	455	ALA
1	B	382	SER
1	A	255	LYS
1	A	421	VAL
1	B	375	GLY
1	B	431	SER
1	B	305	GLY
1	A	61	GLY

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Mol	Chain	Res	Type
1	A	179	GLY
1	A	329	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	394/414 (95%)	338 (86%)	56 (14%)	3 16
1	B	385/414 (93%)	315 (82%)	70 (18%)	1 9
All	All	779/828 (94%)	653 (84%)	126 (16%)	2 12

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	23	LEU
1	A	25	SER
1	A	31	PHE
1	A	33	ARG
1	A	34	ASN
1	A	35	LEU
1	A	44	MET
1	A	45	ARG
1	A	63	THR
1	A	72	LEU
1	A	73	VAL
1	A	84	LEU
1	A	87	ILE
1	A	100	THR
1	A	104	SER
1	A	113	GLN
1	A	126	ILE
1	A	130	SER
1	A	131	LYS
1	A	136	ILE

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Mol	Chain	Res	Type
1	A	138	ASN
1	A	142	LYS
1	A	184	ASN
1	A	221	SER
1	A	222	CYS
1	A	227	LYS
1	A	236	LYS
1	A	252	ARG
1	A	260	ARG
1	A	273	VAL
1	A	280	SER
1	A	290	GLU
1	A	295	LYS
1	A	296	ASP
1	A	297	VAL
1	A	300	ARG
1	A	301	LYS
1	A	302	LEU
1	A	307	ASP
1	A	309	VAL
1	A	320	GLU
1	A	330	SER
1	A	358	VAL
1	A	376	LYS
1	A	379	ARG
1	A	384	ARG
1	A	387	ILE
1	A	393	ARG
1	A	396	SER
1	A	419	VAL
1	A	421	VAL
1	A	439	THR
1	A	449	ASP
1	A	457	TRP
1	A	465	ASP
1	B	8	GLU
1	B	23	LEU
1	B	24	ARG
1	B	37	ARG
1	B	40	GLN
1	B	58	GLU
1	B	59	PHE

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Mol	Chain	Res	Type
1	B	70	SER
1	B	72	LEU
1	B	84	LEU
1	B	92	GLN
1	B	95	THR
1	B	97	GLU
1	B	100	THR
1	B	113	GLN
1	B	116	ASN
1	B	126	ILE
1	B	130	SER
1	B	131	LYS
1	B	134	SER
1	B	135	THR
1	B	143	VAL
1	B	155	PHE
1	B	166	GLU
1	B	170	LYS
1	B	180	ASP
1	B	184	ASN
1	B	185	ARG
1	B	191	ILE
1	B	195	ASP
1	B	197	ILE
1	B	200	VAL
1	B	216	LEU
1	B	219	ASP
1	B	236	LYS
1	B	247	THR
1	B	251	LYS
1	B	252	ARG
1	B	262	ILE
1	B	267	ARG
1	B	273	VAL
1	B	277	ARG
1	B	280	SER
1	B	286	LEU
1	B	288	GLN
1	B	293	ASN
1	B	296	ASP
1	B	298	ARG
1	B	301	LYS

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Mol	Chain	Res	Type
1	B	302	LEU
1	B	309	VAL
1	B	338	ILE
1	B	339	LYS
1	B	342	VAL
1	B	348	ILE
1	B	370	ARG
1	B	376	LYS
1	B	385	VAL
1	B	402	THR
1	B	410	LEU
1	B	414	SER
1	B	417	ILE
1	B	434	ARG
1	B	438	SER
1	B	439	THR
1	B	443	SER
1	B	450	ASN
1	B	457	TRP
1	B	460	SER
1	B	462	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	92	GLN
1	A	113	GLN
1	A	138	ASN
1	A	293	ASN
1	A	345	ASN
1	B	55	GLN
1	B	113	GLN
1	B	116	ASN
1	B	211	GLN
1	B	357	GLN
1	B	386	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	449/470 (95%)	-0.05	6 (1%)	77	51	14, 31, 60, 87	0
1	B	437/470 (92%)	-0.08	3 (0%)	87	69	16, 34, 60, 77	0
All	All	886/940 (94%)	-0.06	9 (1%)	82	59	14, 33, 60, 87	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	GLY	4.2
1	A	305	GLY	3.5
1	A	296	ASP	3.4
1	A	297	VAL	2.9
1	B	114	SER	2.5
1	A	304	PRO	2.4
1	B	113	GLN	2.3
1	B	297	VAL	2.3
1	A	36	ASP	2.1

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.