Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 02:54 AM EDT

PDB ID	:	3K46
Title	:	Crystal structure of full-length E. coli beta-glucuronidase
Authors	:	Wallace, B.D.; Lane, K.T.; Redinbo, M.R.
Deposited on	:	2009-10-05
Resolution	:	2.50 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:

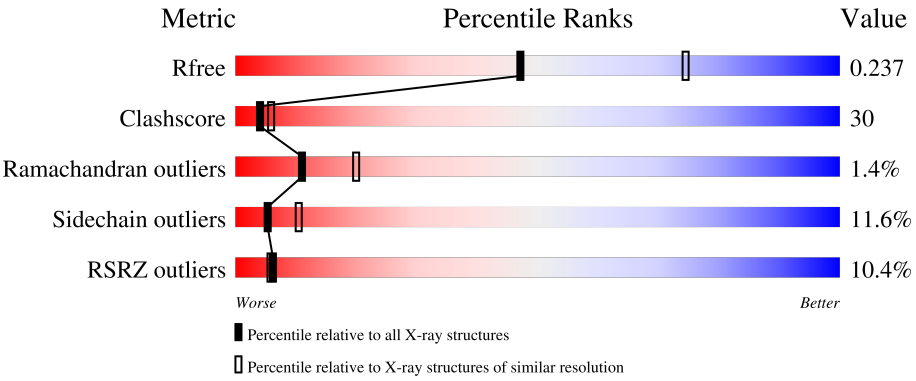
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	605	6% 58% 32% 8% .
1	B	605	14% 54% 35% 8% ..

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9918 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4781	3035	826	898	22			
1	B	596	Total	C	N	O	S	0	0	0
			4780	3034	826	898	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P05804
A	0	HIS	-	expression tag	UNP P05804
B	-1	SER	-	expression tag	UNP P05804
B	0	HIS	-	expression tag	UNP P05804

- Molecule 2 is water.

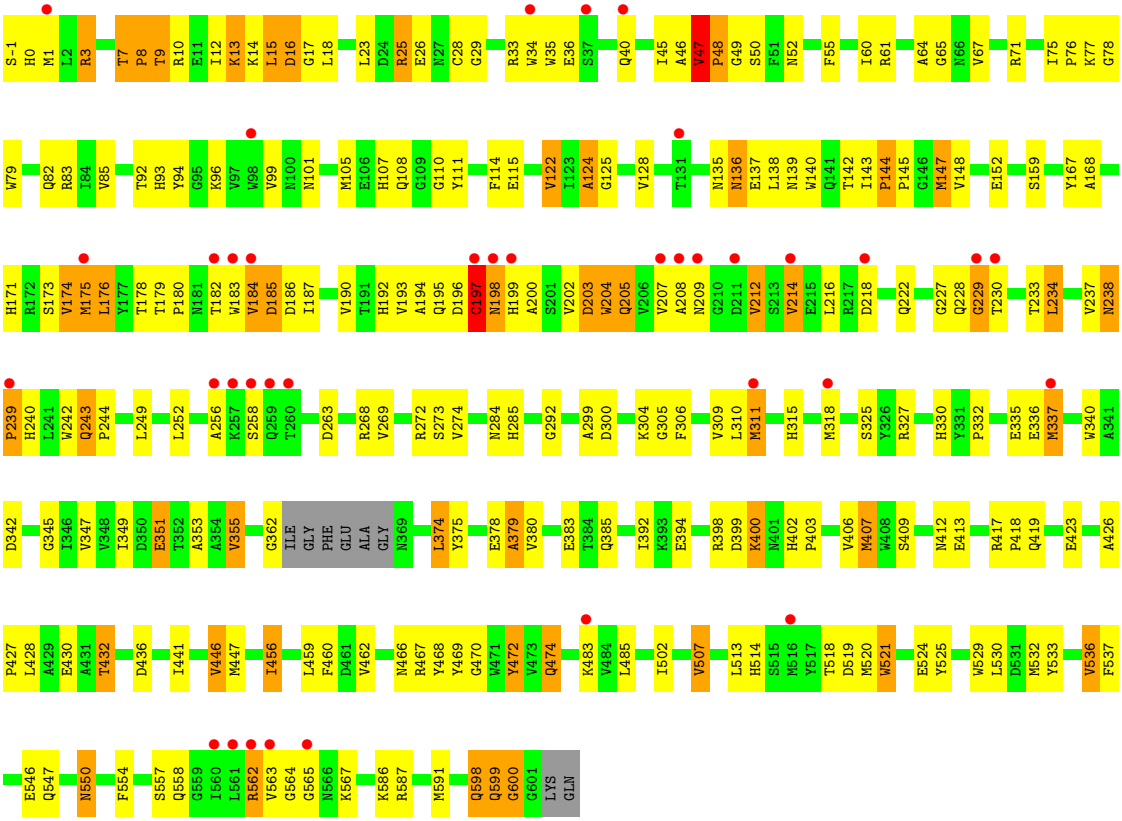
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	245	Total	O	0	0
			245	245		
2	B	112	Total	O	0	0
			112	112		

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.

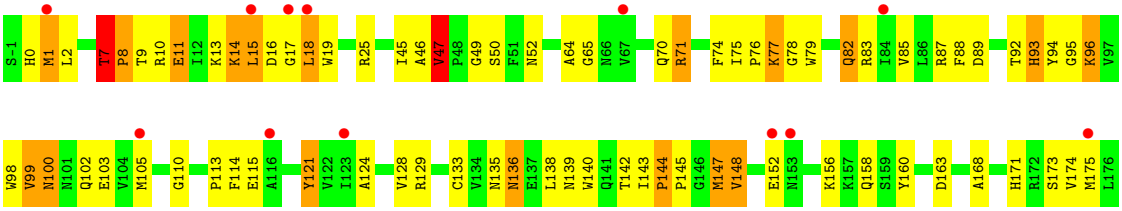
• Molecule 1: Beta-glucuronidase

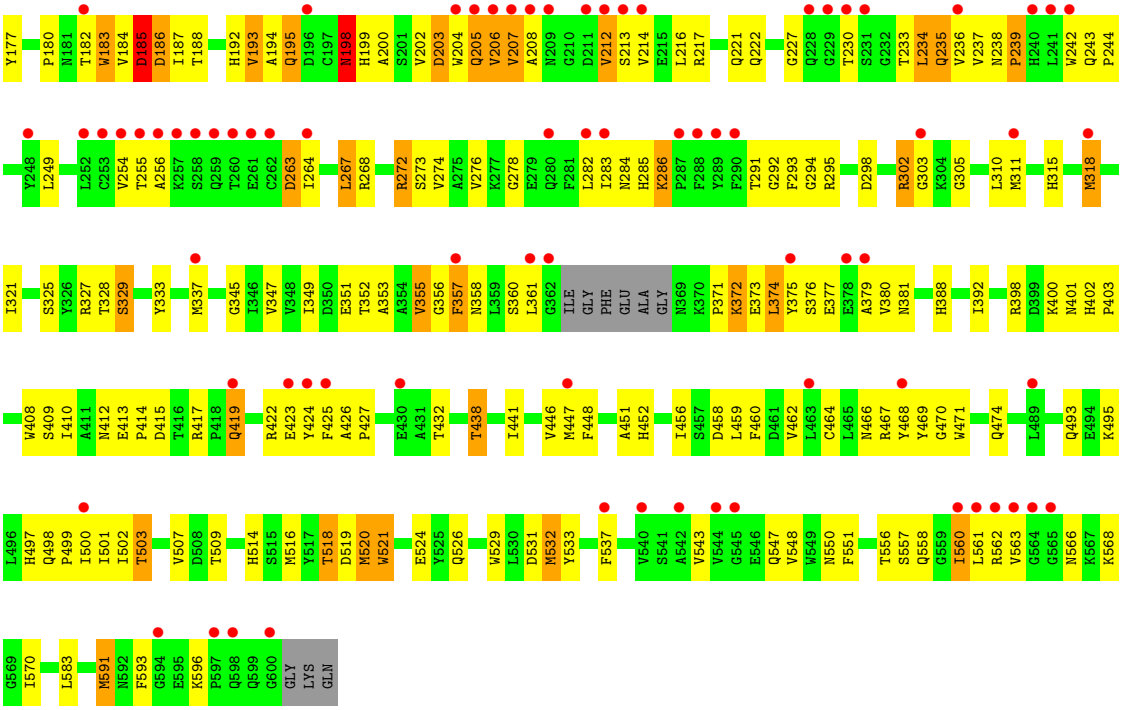
Chain A:



• Molecule 1: Beta-glucuronidase

Chain B:




Y177 P180 N181 T182 W183 V184 D185 D186 I187 T188 H192 V193 A194 Q195 D196 C197 N198 H199 A200 S201 V202 D203 W204 Q205 V206 V207 A208 N209 G210 D211 V212 S213 V214 E215 L216 R217 Q221 Q222 G227 Q228 G229 T230 S231 G232 T233 L234 Q235 V236 V237 N238 P239 H240 L241 W242 Q243 P244
Y248 L249 L252 C253 V254 T255 A256 K257 S258 Q259 T260 E261 C262 D263 I264 L267 R268 R272 S273 V274 A275 V276 K277 G278 E279 Q280 F281 L282 I283 N284 H285 K286 P287 P288 Y289 F290 T291 G292 F293 G294 R295 D298 R302 G303 K304 G305 L310 M311 H315 M318
I321 S325 Y326 R327 T328 S329 Y333 M337 G345 I346 V347 V348 I349 D350 E351 T352 A353 A354 V355 G356 F357 N358 L359 S360 L361 G362 ILE GLY PHE GLU ALA GLY N369 K370 P371 K372 E373 L374 Y375 S376 E377 E378 A379 V380 N381 H388 I392 R398 D399 K400 N401 H402 P403
W408 S409 I410 A411 N412 E413 P414 D415 T416 R417 P418 Q419 R422 E423 Y424 F425 A426 P427 E430 A431 T432 T438 I441 V446 M447 F448 A451 H452 I456 S457 D458 L459 F460 D461 V462 L463 C464 L465 N466 R467 Y468 Y469 G470 W471 Q474 L489 Q493 E494 K495
L496 H497 Q498 P499 I500 I501 I502 T503 V507 D508 T509 H514 S515 M516 Y517 T518 D519 M520 W521 E524 Y525 Q526 W529 L530 D531 M532 Y533 F537 V540 S541 A542 V543 V544 G545 E546 Q547 V548 W549 N550 F551 T556 S557 Q558 G559 I560 L561 R562 V563 G564 G565 N566 K567 K568
G569 I570 L583 M591 N592 F593 G594 E595 K596 P597 Q598 Q599 G600 GLY LYS GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.75Å 76.19Å 125.67Å 90.00° 125.00° 90.00°	Depositor
Resolution (Å)	30.62 – 2.50 47.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.62-2.50) 95.5 (47.63-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.267 0.212 , 0.237	Depositor DCC
R_{free} test set	2206 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9918	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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	0.63	10/4909 (0.2%)	0.69	9/6680 (0.1%)
1	B	0.55	8/4908 (0.2%)	0.66	5/6679 (0.1%)
All	All	0.59	18/9817 (0.2%)	0.67	14/13359 (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	5
1	B	0	2
All	All	0	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	520	MET	CG-SD	6.37	1.97	1.81
1	B	516	MET	CG-SD	6.34	1.97	1.81
1	B	591	MET	CG-SD	6.33	1.97	1.81
1	A	532	MET	CG-SD	6.11	1.97	1.81
1	B	532	MET	CG-SD	6.08	1.97	1.81
1	B	147	MET	CG-SD	5.91	1.96	1.81
1	A	407	MET	CG-SD	5.87	1.96	1.81
1	A	337	MET	CG-SD	5.87	1.96	1.81
1	A	311	MET	CG-SD	5.86	1.96	1.81
1	A	175	MET	CG-SD	5.82	1.96	1.81
1	A	1	MET	CG-SD	5.73	1.96	1.81
1	B	318	MET	CG-SD	5.61	1.95	1.81
1	B	1	MET	CG-SD	5.48	1.95	1.81
1	A	147	MET	CG-SD	5.47	1.95	1.81
1	B	520	MET	CG-SD	5.46	1.95	1.81
1	B	337	MET	CG-SD	5.46	1.95	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	MET	CG-SD	5.26	1.94	1.81
1	A	591	MET	CG-SD	5.08	1.94	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	185	ASP	N-CA-C	8.18	133.09	111.00
1	B	198	ASN	N-CA-C	7.56	131.40	111.00
1	B	198	ASN	N-CA-CB	-7.17	97.70	110.60
1	B	185	ASP	N-CA-CB	-6.38	99.12	110.60
1	A	300	ASP	N-CA-C	5.94	127.04	111.00
1	A	380	VAL	N-CA-C	-5.75	95.48	111.00
1	A	197	CYS	N-CA-C	-5.65	95.73	111.00
1	A	379	ALA	N-CA-C	5.62	126.17	111.00
1	A	16	ASP	N-CA-C	-5.60	95.87	111.00
1	A	550	ASN	N-CA-C	5.39	125.55	111.00
1	A	108	GLN	N-CA-C	5.35	125.45	111.00
1	A	185	ASP	N-CA-C	5.33	125.40	111.00
1	B	100	ASN	CB-CA-C	5.32	121.04	110.40
1	A	48	PRO	N-CA-C	-5.11	98.81	112.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ILE	Mainchain,Peptide
1	A	184	VAL	Peptide
1	A	47	VAL	Mainchain,Peptide
1	B	143	ILE	Peptide
1	B	47	VAL	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	4781	0	4560	249	0
1	B	4780	0	4561	319	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	245	0	0	30	0
2	B	112	0	0	15	0
All	All	9918	0	9121	560	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 30.

All (560) 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:207:VAL:HG21	1:A:212:VAL:CG1	1.35	1.51
1:B:283:ILE:O	1:B:286:LYS:HD3	1.25	1.35
1:A:207:VAL:CG2	1:A:212:VAL:HG11	1.65	1.25
1:B:183:TRP:CD2	1:B:207:VAL:HG11	1.79	1.18
1:A:407:MET:HE2	2:A:833:HOH:O	1.04	1.18
1:A:207:VAL:CG2	1:A:212:VAL:CG1	2.23	1.16
1:B:205:GLN:OE1	1:B:207:VAL:HG22	1.46	1.16
1:A:207:VAL:HG21	1:A:212:VAL:HG12	1.12	1.08
1:B:17:GLY:O	1:B:46:ALA:HA	1.53	1.06
1:B:198:ASN:HB2	1:B:237:VAL:O	1.58	1.03
1:A:207:VAL:HG21	1:A:212:VAL:HG11	1.12	1.02
1:B:183:TRP:CG	1:B:207:VAL:HG11	1.95	1.01
1:B:194:ALA:O	2:B:655:HOH:O	1.78	1.00
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.25	1.00
1:B:263:ASP:OD2	2:B:658:HOH:O	1.81	0.99
1:A:-1:SER:O	2:A:687:HOH:O	1.80	0.99
1:B:286:LYS:HE2	1:B:286:LYS:O	1.61	0.98
1:A:239:PRO:HD2	2:A:697:HOH:O	1.64	0.96
1:B:286:LYS:HE2	1:B:286:LYS:N	1.82	0.95
1:B:183:TRP:CD1	1:B:184:VAL:O	2.21	0.94
1:B:286:LYS:HE2	1:B:286:LYS:H	1.32	0.94
1:A:25:ARG:HG3	1:A:25:ARG:HH11	1.34	0.93
1:B:195:GLN:NE2	1:B:195:GLN:HA	1.84	0.93
1:A:362:GLY:O	2:A:758:HOH:O	1.86	0.92
1:B:283:ILE:O	1:B:286:LYS:CD	2.16	0.92
1:A:175:MET:HE3	2:A:834:HOH:O	1.68	0.91
1:A:407:MET:CE	2:A:833:HOH:O	1.71	0.91
1:B:198:ASN:CB	1:B:237:VAL:O	2.19	0.91
1:B:183:TRP:CG	1:B:207:VAL:CG1	2.55	0.89
1:B:138:LEU:HD22	1:B:142:THR:HG21	1.54	0.89
1:A:175:MET:CE	2:A:834:HOH:O	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:O	2:A:832:HOH:O	1.91	0.87
1:B:286:LYS:O	1:B:286:LYS:CE	2.23	0.87
1:A:-1:SER:C	2:A:687:HOH:O	2.10	0.87
1:B:285:HIS:N	1:B:286:LYS:NZ	2.23	0.86
1:B:283:ILE:H	1:B:286:LYS:HE3	1.37	0.86
1:B:198:ASN:HD21	1:B:236:VAL:HG12	1.42	0.85
1:A:202:VAL:HG13	2:A:744:HOH:O	1.75	0.84
1:A:243:GLN:HE21	1:A:243:GLN:HA	1.41	0.84
1:A:311:MET:HE3	1:A:337:MET:HA	1.57	0.84
1:B:198:ASN:CG	1:B:237:VAL:O	2.16	0.84
1:A:207:VAL:CG1	1:A:256:ALA:CB	2.57	0.82
1:A:187:ILE:HA	1:A:205:GLN:HB2	1.61	0.82
1:B:183:TRP:CD2	1:B:207:VAL:CG1	2.62	0.81
1:B:374:LEU:O	1:B:380:VAL:HG12	1.80	0.81
1:B:283:ILE:N	1:B:286:LYS:HE3	1.94	0.81
1:A:207:VAL:CG1	1:A:256:ALA:HB1	2.11	0.80
1:A:199:HIS:CD2	1:A:200:ALA:H	2.00	0.80
1:B:205:GLN:CD	1:B:207:VAL:HG22	2.02	0.79
1:B:286:LYS:HE2	1:B:286:LYS:CA	2.13	0.79
1:B:186:ASP:HB3	1:B:206:VAL:HG13	1.63	0.78
1:B:272:ARG:HA	1:B:284:ASN:OD1	1.85	0.77
1:B:142:THR:HG22	1:B:144:PRO:O	1.85	0.76
1:A:207:VAL:HG11	1:A:256:ALA:CB	2.16	0.76
1:B:0:HIS:HB2	1:B:185:ASP:HB2	1.67	0.75
1:B:286:LYS:HE2	1:B:286:LYS:C	2.06	0.75
1:B:14:LYS:HB3	1:B:14:LYS:HZ2	1.51	0.75
1:A:192:HIS:O	1:A:199:HIS:HB3	1.87	0.75
1:B:285:HIS:N	1:B:286:LYS:HZ2	1.85	0.74
1:A:139:ASN:O	1:A:142:THR:HG22	1.87	0.74
1:B:212:VAL:CG2	1:B:230:THR:HA	2.17	0.74
1:A:207:VAL:HG11	1:A:256:ALA:HB1	1.69	0.74
1:A:311:MET:HE1	1:A:340:TRP:HB2	1.70	0.74
1:A:194:ALA:O	2:A:627:HOH:O	2.06	0.73
1:B:193:VAL:O	1:B:285:HIS:NE2	2.19	0.73
1:B:52:ASN:HD21	1:B:168:ALA:H	1.37	0.73
1:A:207:VAL:CG2	1:A:212:VAL:HG12	2.06	0.73
1:B:193:VAL:HG13	1:B:273:SER:HB3	1.71	0.73
1:A:23:LEU:HD11	1:A:60:ILE:HG12	1.69	0.72
1:A:52:ASN:HD21	1:A:168:ALA:H	1.37	0.72
1:A:182:THR:O	1:A:208:ALA:O	2.06	0.72
1:B:285:HIS:N	1:B:286:LYS:HZ3	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:H	1:A:110:GLY:CA	2.03	0.72
1:A:140:TRP:HB3	1:A:379:ALA:O	1.91	0.71
1:B:212:VAL:HG22	1:B:230:THR:HA	1.73	0.71
1:A:351:GLU:HG2	1:A:409:SER:HB3	1.73	0.71
1:B:140:TRP:HB3	1:B:379:ALA:O	1.91	0.71
1:A:207:VAL:HG23	1:A:212:VAL:HG11	1.71	0.70
1:A:82:GLN:HA	1:A:82:GLN:OE1	1.90	0.70
1:B:184:VAL:HG12	1:B:185:ASP:H	1.55	0.70
1:B:192:HIS:O	1:B:199:HIS:HB3	1.90	0.70
1:A:554:PHE:O	1:A:565:GLY:O	2.09	0.70
1:B:283:ILE:N	1:B:286:LYS:CE	2.54	0.70
1:A:13:LYS:HG3	1:A:15:LEU:HD21	1.72	0.70
1:B:7:THR:HB	1:B:8:PRO:HD2	1.72	0.70
1:A:25:ARG:HH11	1:A:25:ARG:CG	2.04	0.70
1:B:203:ASP:CG	1:B:233:THR:HB	2.11	0.70
1:B:237:VAL:HG22	1:B:238:ASN:H	1.55	0.70
1:A:192:HIS:HB2	1:A:199:HIS:CD2	2.26	0.70
1:A:507:VAL:HG22	1:A:529:TRP:CD1	2.26	0.70
1:A:412:ASN:HD21	1:A:466:ASN:HD21	1.39	0.70
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.00	0.70
1:A:0:HIS:ND1	1:A:186:ASP:HB2	2.07	0.70
1:B:203:ASP:HB3	1:B:233:THR:HB	1.74	0.69
1:B:392:ILE:HG21	1:B:432:THR:HG21	1.74	0.69
1:B:94:TYR:HB3	1:B:135:ASN:HB3	1.74	0.69
1:B:200:ALA:HB1	1:B:234:LEU:CD2	2.23	0.69
1:A:207:VAL:CG1	1:A:256:ALA:HB2	2.21	0.69
1:B:244:PRO:HB2	1:B:593:PHE:HE1	1.57	0.69
1:B:286:LYS:H	1:B:286:LYS:CE	2.06	0.69
1:B:205:GLN:HE22	1:B:207:VAL:CG2	2.07	0.68
1:B:193:VAL:HA	1:B:199:HIS:HB3	1.75	0.68
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.75	0.67
1:A:311:MET:CE	1:A:340:TRP:HB2	2.23	0.67
1:A:202:VAL:HG22	1:A:234:LEU:CD2	2.25	0.67
1:B:198:ASN:ND2	1:B:236:VAL:HG12	2.09	0.67
1:B:471:TRP:CD1	1:B:507:VAL:HG12	2.30	0.67
1:B:286:LYS:N	1:B:286:LYS:CE	2.55	0.67
1:B:328:THR:O	1:B:351:GLU:HB3	1.94	0.67
1:A:198:ASN:HB3	1:A:237:VAL:O	1.95	0.67
1:A:-1:SER:CA	2:A:687:HOH:O	2.41	0.66
1:B:452:HIS:ND1	2:B:619:HOH:O	2.29	0.66
1:B:375:TYR:HA	1:B:380:VAL:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LYS:HB3	1:B:14:LYS:NZ	2.09	0.65
1:B:93:HIS:H	1:B:110:GLY:CA	2.09	0.65
1:B:548:VAL:HG11	1:B:570:ILE:HD11	1.79	0.65
1:A:35:TRP:HD1	1:A:101:ASN:HA	1.62	0.65
1:B:200:ALA:HA	1:B:235:GLN:O	1.97	0.65
1:A:485:LEU:HD23	1:A:536:VAL:HG11	1.79	0.65
1:B:15:LEU:HD13	1:B:15:LEU:O	1.97	0.65
1:B:244:PRO:HB2	1:B:593:PHE:CE1	2.32	0.65
1:B:284:ASN:C	1:B:286:LYS:HZ2	1.99	0.65
1:A:342:ASP:OD2	1:A:402:HIS:HD2	1.79	0.64
1:A:598:GLN:CD	1:A:598:GLN:H	2.00	0.64
1:B:185:ASP:N	1:B:185:ASP:OD1	2.30	0.64
1:B:402:HIS:NE2	2:B:625:HOH:O	2.30	0.64
1:A:207:VAL:HG13	1:A:256:ALA:HB2	1.78	0.64
1:B:203:ASP:CB	1:B:233:THR:HB	2.27	0.64
1:B:507:VAL:HG13	1:B:529:TRP:CD1	2.33	0.64
1:A:105:MET:CE	1:A:115:GLU:HA	2.28	0.63
1:B:193:VAL:HA	1:B:199:HIS:CB	2.28	0.63
1:B:2:LEU:HG	1:B:185:ASP:O	1.99	0.63
1:B:183:TRP:NE1	1:B:184:VAL:O	2.30	0.63
1:B:282:LEU:HA	1:B:286:LYS:HE3	1.80	0.63
1:B:447:MET:HE1	1:B:470:GLY:HA2	1.80	0.63
1:A:392:ILE:HG21	1:A:432:THR:HG22	1.81	0.62
1:B:284:ASN:N	1:B:286:LYS:HZ2	1.97	0.62
1:B:502:ILE:HG13	1:B:537:PHE:CE2	2.34	0.62
1:A:436:ASP:O	2:A:757:HOH:O	2.15	0.62
1:A:23:LEU:HD23	1:A:67:VAL:HG12	1.82	0.62
1:A:93:HIS:H	1:A:110:GLY:HA2	1.64	0.62
1:B:560:ILE:HD12	1:B:560:ILE:H	1.65	0.62
1:A:193:VAL:HG23	1:A:285:HIS:NE2	2.15	0.62
1:A:249:LEU:HD13	1:A:268:ARG:HE	1.63	0.62
1:B:7:THR:HB	1:B:8:PRO:CD	2.29	0.62
1:A:502:ILE:HG13	1:A:537:PHE:CE2	2.34	0.61
1:A:355:VAL:HG13	1:A:412:ASN:HB3	1.81	0.61
1:B:425:PHE:CB	1:B:456:ILE:HD11	2.31	0.61
1:A:26:GLU:HB2	1:A:28:CYS:SG	2.40	0.61
1:A:33:ARG:NH1	2:A:805:HOH:O	2.33	0.61
1:A:228:GLN:O	1:A:229:GLY:C	2.39	0.61
1:B:556:THR:OG1	1:B:562:ARG:HG3	2.01	0.61
1:A:186:ASP:O	1:A:205:GLN:HB2	2.01	0.60
1:B:243:GLN:HA	1:B:243:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:MET:HA	1:B:321:ILE:HG22	1.83	0.60
1:A:77:LYS:HG3	1:A:125:GLY:HA2	1.81	0.60
1:A:105:MET:HE3	1:A:115:GLU:HA	1.83	0.60
1:A:10:ARG:HH21	1:B:76:PRO:HB3	1.66	0.60
1:A:183:TRP:CD1	1:A:184:VAL:N	2.70	0.60
1:A:207:VAL:HG12	1:A:207:VAL:O	2.00	0.60
1:A:514:HIS:HD2	1:A:524:GLU:OE1	1.83	0.60
1:A:107:HIS:HE1	1:A:394:GLU:OE1	1.84	0.60
1:B:238:ASN:HB3	1:B:239:PRO:HD2	1.84	0.60
1:B:243:GLN:NE2	1:B:284:ASN:HD22	1.99	0.60
1:B:192:HIS:NE2	1:B:202:VAL:HG23	2.17	0.60
1:B:283:ILE:C	1:B:286:LYS:HD3	2.17	0.60
1:A:13:LYS:HG3	1:A:15:LEU:CD2	2.31	0.60
1:A:202:VAL:HG22	1:A:234:LEU:HD23	1.82	0.60
1:B:147:MET:HE1	1:B:371:PRO:HD2	1.83	0.60
1:A:428:LEU:O	1:A:432:THR:HG23	2.02	0.59
1:A:218:ASP:HB2	1:A:222:GLN:HG2	1.84	0.59
1:B:82:GLN:CD	1:B:82:GLN:H	2.03	0.59
1:B:203:ASP:OD1	1:B:214:VAL:HG11	2.01	0.59
1:B:422:ARG:NH2	1:B:458:ASP:OD1	2.35	0.59
1:A:142:THR:HG23	1:A:144:PRO:O	2.01	0.59
1:B:285:HIS:H	1:B:286:LYS:NZ	1.99	0.59
1:A:468:TYR:O	1:A:469:TYR:HB2	2.02	0.59
1:B:200:ALA:HB1	1:B:234:LEU:HD23	1.85	0.59
1:B:282:LEU:HB3	1:B:286:LYS:NZ	2.18	0.59
1:B:413:GLU:HB3	1:B:446:VAL:HG22	1.84	0.59
1:A:299:ALA:CB	1:A:310:LEU:HD11	2.32	0.59
1:A:502:ILE:HG13	1:A:537:PHE:CZ	2.37	0.59
1:A:17:GLY:CA	1:A:47:VAL:H	2.15	0.59
1:B:205:GLN:NE2	1:B:207:VAL:HG22	2.17	0.59
1:B:180:PRO:HD3	2:B:697:HOH:O	2.02	0.58
1:A:349:ILE:HG12	1:A:407:MET:HE3	1.85	0.58
1:B:242:TRP:CZ2	1:B:345:GLY:HA2	2.39	0.58
1:B:283:ILE:C	1:B:286:LYS:NZ	2.57	0.58
1:A:398:ARG:HD2	1:A:399:ASP:OD1	2.04	0.58
1:B:18:LEU:HA	1:B:45:ILE:O	2.03	0.58
1:A:139:ASN:H	1:A:142:THR:CG2	2.16	0.58
1:A:76:PRO:O	1:A:79:TRP:HB2	2.04	0.57
1:A:139:ASN:H	1:A:142:THR:HG22	1.68	0.57
1:B:214:VAL:HG12	1:B:214:VAL:O	2.03	0.57
1:B:14:LYS:C	1:B:16:ASP:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:NH1	1:B:503:THR:HB	2.19	0.57
1:A:243:GLN:NE2	1:A:284:ASN:HD22	2.02	0.57
1:B:212:VAL:HA	1:B:255:THR:O	2.03	0.57
1:A:249:LEU:O	2:A:690:HOH:O	2.18	0.57
1:B:195:GLN:HA	1:B:195:GLN:HE21	1.66	0.57
1:B:227:GLY:HA3	1:B:233:THR:CG2	2.34	0.57
1:B:238:ASN:HB3	1:B:239:PRO:CD	2.35	0.57
1:B:14:LYS:HB2	1:B:71:ARG:HE	1.69	0.57
1:B:183:TRP:CD1	1:B:207:VAL:CG1	2.87	0.57
1:B:311:MET:O	1:B:315:HIS:HD2	1.88	0.57
1:A:35:TRP:CD1	1:A:101:ASN:HA	2.40	0.57
1:A:94:TYR:OH	1:A:96:LYS:HE3	2.05	0.57
1:B:138:LEU:HD22	1:B:142:THR:CG2	2.29	0.57
1:B:205:GLN:NE2	1:B:207:VAL:CG2	2.67	0.57
1:B:222:GLN:NE2	2:B:691:HOH:O	2.38	0.57
1:B:283:ILE:N	1:B:286:LYS:HZ1	2.02	0.56
1:B:148:VAL:HG12	1:B:158:GLN:OE1	2.06	0.56
1:B:198:ASN:HD21	1:B:236:VAL:CG1	2.14	0.56
1:B:188:THR:HB	1:B:204:TRP:HB3	1.87	0.56
1:B:292:GLY:HA3	1:B:325:SER:O	2.05	0.56
1:A:184:VAL:HG12	1:A:185:ASP:HB3	1.88	0.56
1:A:470:GLY:O	1:A:474:GLN:HB2	2.05	0.56
1:A:309:VAL:HG23	2:A:638:HOH:O	2.06	0.56
1:B:200:ALA:HB1	1:B:234:LEU:HD21	1.86	0.56
1:A:244:PRO:O	1:A:345:GLY:O	2.24	0.56
1:B:75:ILE:O	1:B:124:ALA:O	2.24	0.56
1:B:283:ILE:C	1:B:286:LYS:HZ2	2.09	0.56
1:A:77:LYS:HZ1	1:B:8:PRO:HA	1.71	0.56
1:A:183:TRP:CD1	1:A:207:VAL:HA	2.41	0.56
1:B:267:LEU:HG	1:B:268:ARG:N	2.21	0.56
1:A:193:VAL:HG23	1:A:285:HIS:HE2	1.69	0.55
1:B:1:MET:HE3	1:B:1:MET:HA	1.88	0.55
1:B:70:GLN:NE2	1:B:129:ARG:HD2	2.22	0.55
1:B:89:ASP:OD2	1:B:173:SER:HB2	2.05	0.55
1:B:441:ILE:HG22	1:B:460:PHE:HD1	1.71	0.55
1:A:10:ARG:HH11	1:B:77:LYS:HE2	1.72	0.55
1:A:17:GLY:HA3	1:A:47:VAL:H	1.70	0.55
1:A:564:GLY:HA2	2:A:625:HOH:O	2.06	0.55
1:B:282:LEU:C	1:B:286:LYS:HZ1	2.09	0.55
1:A:10:ARG:NH2	1:B:76:PRO:HB3	2.22	0.55
1:A:49:GLY:HA2	1:A:305:GLY:HA3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:TRP:CG	1:B:207:VAL:HG12	2.41	0.55
1:A:36:GLU:HA	1:A:101:ASN:OD1	2.07	0.55
1:A:65:GLY:H	1:A:136:ASN:HD21	1.55	0.54
1:A:447:MET:HE1	1:A:470:GLY:HA2	1.90	0.54
1:B:283:ILE:H	1:B:286:LYS:CE	2.09	0.54
1:B:351:GLU:HA	1:B:409:SER:HB3	1.89	0.54
1:B:468:TYR:O	1:B:469:TYR:HB2	2.08	0.54
1:A:468:TYR:HA	2:A:803:HOH:O	2.07	0.54
1:A:77:LYS:NZ	1:B:8:PRO:HA	2.22	0.54
1:B:83:ARG:HH12	1:B:184:VAL:HA	1.71	0.54
1:A:50:SER:HB3	1:A:52:ASN:HD22	1.73	0.54
1:A:413:GLU:HB3	1:A:446:VAL:HG13	1.89	0.54
1:B:105:MET:HE1	1:B:114:PHE:O	2.08	0.54
1:B:205:GLN:NE2	1:B:212:VAL:HG11	2.22	0.54
1:A:204:TRP:CD1	1:A:204:TRP:C	2.81	0.53
1:B:7:THR:C	1:B:9:THR:H	2.11	0.53
1:B:273:SER:O	1:B:283:ILE:HA	2.07	0.53
1:B:413:GLU:CB	1:B:446:VAL:HG22	2.38	0.53
1:A:187:ILE:HA	1:A:205:GLN:CB	2.37	0.53
1:B:19:TRP:CZ2	1:B:174:VAL:HG11	2.43	0.53
1:B:388:HIS:CD2	1:B:392:ILE:HD11	2.44	0.53
1:B:82:GLN:CD	1:B:82:GLN:N	2.62	0.53
1:B:93:HIS:H	1:B:110:GLY:HA3	1.73	0.53
1:B:388:HIS:O	1:B:392:ILE:HG13	2.08	0.53
1:A:3:ARG:CZ	1:A:335:GLU:HG3	2.38	0.53
1:A:93:HIS:H	1:A:110:GLY:HA3	1.74	0.53
1:A:29:GLY:HA2	1:A:34:TRP:CE2	2.44	0.53
1:A:193:VAL:HG22	1:A:273:SER:HB3	1.89	0.53
1:B:0:HIS:HB2	1:B:185:ASP:CB	2.39	0.52
1:A:25:ARG:CG	1:A:25:ARG:NH1	2.71	0.52
1:B:212:VAL:HG21	1:B:230:THR:HA	1.90	0.52
1:B:283:ILE:N	1:B:286:LYS:NZ	2.58	0.52
1:A:52:ASN:ND2	1:A:52:ASN:H	2.08	0.52
1:A:204:TRP:HD1	1:A:205:GLN:N	2.07	0.52
1:B:413:GLU:CA	1:B:446:VAL:HG22	2.40	0.52
1:A:426:ALA:HA	1:A:459:LEU:HD13	1.91	0.52
1:B:138:LEU:CD2	1:B:142:THR:HG21	2.33	0.52
1:B:187:ILE:CG2	1:B:188:THR:N	2.73	0.52
1:A:203:ASP:OD2	1:A:203:ASP:C	2.48	0.52
1:B:183:TRP:CE3	1:B:207:VAL:HG11	2.39	0.52
1:A:10:ARG:CZ	1:A:79:TRP:HE1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH2	1:A:184:VAL:HG11	2.24	0.51
1:A:529:TRP:CE2	1:A:533:TYR:HE1	2.29	0.51
1:B:412:ASN:HD21	1:B:466:ASN:HD21	1.57	0.51
1:A:0:HIS:HB3	1:A:185:ASP:O	2.11	0.51
1:A:82:GLN:HG3	1:A:178:THR:HG23	1.91	0.51
1:A:65:GLY:HA2	1:A:137:GLU:OE2	2.10	0.51
1:A:82:GLN:O	1:A:179:THR:O	2.29	0.51
1:A:342:ASP:CG	1:A:403:PRO:HD2	2.31	0.51
1:A:529:TRP:NE1	1:A:533:TYR:HE1	2.08	0.51
1:A:547:GLN:NE2	2:A:648:HOH:O	2.41	0.51
1:B:15:LEU:O	1:B:15:LEU:CD1	2.59	0.51
1:A:29:GLY:HA2	1:A:34:TRP:CD2	2.45	0.51
1:A:76:PRO:HD2	1:A:79:TRP:CE3	2.46	0.51
1:B:79:TRP:O	1:B:82:GLN:HG2	2.10	0.51
1:B:105:MET:HE3	1:B:115:GLU:HA	1.92	0.51
1:A:417:ARG:N	1:A:418:PRO:CD	2.74	0.51
1:B:10:ARG:CZ	1:B:79:TRP:HE1	2.24	0.51
1:A:227:GLY:HA3	1:A:233:THR:HG21	1.92	0.51
1:A:306:PHE:CZ	1:A:336:GLU:HG3	2.46	0.50
1:B:284:ASN:O	1:B:286:LYS:HG3	2.10	0.50
1:A:598:GLN:O	1:A:599:GLN:C	2.50	0.50
1:B:227:GLY:HA3	1:B:233:THR:HG23	1.93	0.50
1:B:286:LYS:O	1:B:286:LYS:HE3	2.11	0.50
1:A:10:ARG:HD3	1:B:77:LYS:HE2	1.92	0.50
1:B:14:LYS:C	1:B:16:ASP:N	2.65	0.50
1:B:65:GLY:H	1:B:136:ASN:HD21	1.60	0.50
1:B:351:GLU:OE1	1:B:412:ASN:HB2	2.12	0.50
1:A:92:THR:HA	1:A:110:GLY:HA2	1.94	0.50
1:B:49:GLY:HA2	1:B:305:GLY:HA3	1.94	0.50
1:B:242:TRP:HB2	2:B:662:HOH:O	2.12	0.50
1:A:15:LEU:HD22	1:A:173:SER:CB	2.42	0.50
1:A:140:TRP:CE3	1:A:379:ALA:O	2.64	0.49
1:B:71:ARG:NH1	1:B:71:ARG:CG	2.72	0.49
1:B:358:ASN:HD21	1:B:448:PHE:HZ	1.60	0.49
1:A:14:LYS:HB2	1:A:174:VAL:O	2.11	0.49
1:A:138:LEU:HA	1:A:142:THR:HG21	1.93	0.49
1:B:425:PHE:HB3	1:B:456:ILE:HD11	1.93	0.49
1:A:562:ARG:C	1:A:562:ARG:HD2	2.32	0.49
1:B:291:THR:HG21	1:B:591:MET:HE2	1.93	0.49
1:A:513:LEU:HD23	1:A:521:TRP:O	2.12	0.49
1:B:509:THR:HG21	1:B:526:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:THR:O	1:B:518:THR:OG1	2.29	0.49
1:A:238:ASN:H	1:A:239:PRO:HD3	1.77	0.49
1:B:1:MET:HA	1:B:1:MET:CE	2.42	0.49
1:B:233:THR:HG22	1:B:234:LEU:N	2.28	0.49
1:B:294:GLY:O	1:B:550:ASN:HA	2.12	0.49
1:B:425:PHE:HB2	1:B:456:ILE:HD11	1.95	0.49
1:A:135:ASN:ND2	1:A:137:GLU:H	2.11	0.49
1:A:195:GLN:HG3	2:A:627:HOH:O	2.12	0.49
1:B:186:ASP:O	1:B:187:ILE:HG13	2.13	0.49
1:B:194:ALA:CB	1:B:199:HIS:HD2	2.26	0.49
1:B:377:GLU:HA	1:B:381:ASN:HB3	1.94	0.49
1:B:11:GLU:HB2	1:B:177:TYR:HB3	1.94	0.49
1:B:17:GLY:O	1:B:46:ALA:CA	2.44	0.49
1:B:375:TYR:HA	1:B:380:VAL:CG1	2.42	0.49
1:A:93:HIS:N	1:A:110:GLY:HA2	2.28	0.49
1:A:351:GLU:HG2	1:A:409:SER:CB	2.41	0.49
1:B:293:PHE:CD1	1:B:551:PHE:HA	2.48	0.49
1:B:360:SER:HB2	1:B:417:ARG:HH21	1.78	0.48
1:B:7:THR:C	1:B:9:THR:N	2.66	0.48
1:B:75:ILE:HD11	1:B:128:VAL:HG22	1.95	0.48
1:B:284:ASN:CA	1:B:286:LYS:HZ2	2.26	0.48
1:B:401:ASN:O	1:B:403:PRO:HD3	2.13	0.48
1:B:563:VAL:H	1:B:566:ASN:HA	1.78	0.48
1:A:205:GLN:OE1	1:A:212:VAL:HG21	2.13	0.48
1:B:96:LYS:HD3	1:B:98:TRP:CZ2	2.49	0.48
1:B:102:GLN:HG2	1:B:121:TYR:CG	2.49	0.48
1:A:7:THR:C	1:A:9:THR:N	2.65	0.48
1:A:92:THR:OG1	1:A:171:HIS:ND1	2.42	0.48
1:B:0:HIS:CD2	1:B:185:ASP:OD1	2.65	0.48
1:B:182:THR:O	1:B:208:ALA:O	2.31	0.48
1:B:255:THR:OG1	1:B:264:ILE:HG12	2.13	0.48
1:A:456:ILE:HG23	1:A:460:PHE:HE2	1.77	0.48
1:B:203:ASP:OD2	1:B:203:ASP:C	2.50	0.48
1:B:500:ILE:O	1:B:543:VAL:HA	2.14	0.48
1:A:306:PHE:CE1	1:A:336:GLU:HG3	2.49	0.48
1:A:426:ALA:HB3	1:A:427:PRO:HD3	1.96	0.48
1:B:254:VAL:O	1:B:264:ILE:HA	2.14	0.48
1:B:328:THR:HA	1:B:333:TYR:CZ	2.49	0.48
1:A:200:ALA:HB1	1:A:234:LEU:HD13	1.95	0.48
1:A:327:ARG:NH2	1:A:412:ASN:ND2	2.62	0.48
1:B:207:VAL:HG21	1:B:256:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:THR:OG1	1:B:353:ALA:N	2.47	0.48
1:A:355:VAL:CG1	1:A:412:ASN:HB3	2.44	0.47
1:A:135:ASN:HD21	1:A:137:GLU:HB2	1.79	0.47
1:A:183:TRP:O	1:A:263:ASP:OD2	2.32	0.47
1:B:19:TRP:HZ2	1:B:174:VAL:HG11	1.78	0.47
1:B:351:GLU:HG2	1:B:352:THR:N	2.30	0.47
1:B:562:ARG:HD2	1:B:562:ARG:C	2.34	0.47
1:B:183:TRP:CD1	1:B:207:VAL:HG12	2.49	0.47
1:B:413:GLU:N	1:B:414:PRO:HD3	2.28	0.47
1:A:140:TRP:CD2	1:A:379:ALA:O	2.68	0.47
1:A:122:VAL:HG23	1:A:128:VAL:HG11	1.96	0.47
1:B:194:ALA:HB2	1:B:199:HIS:CD2	2.49	0.47
1:A:92:THR:HA	1:A:110:GLY:CA	2.44	0.47
1:A:204:TRP:CD1	1:A:205:GLN:N	2.82	0.47
1:B:52:ASN:ND2	1:B:168:ALA:H	2.07	0.47
1:B:95:GLY:HA2	1:B:133:CYS:O	2.15	0.47
1:B:193:VAL:CG1	1:B:273:SER:HB3	2.42	0.47
1:B:50:SER:HB2	1:B:303:GLY:HA3	1.97	0.47
1:B:92:THR:HA	1:B:110:GLY:CA	2.44	0.47
1:B:327:ARG:NH2	1:B:412:ASN:ND2	2.63	0.47
1:B:183:TRP:CE2	1:B:207:VAL:CG1	2.97	0.47
1:B:237:VAL:HG22	1:B:238:ASN:N	2.28	0.47
1:A:75:ILE:O	1:A:124:ALA:O	2.33	0.47
1:B:171:HIS:O	1:B:305:GLY:HA2	2.15	0.47
1:A:75:ILE:HD12	1:A:75:ILE:N	2.30	0.47
2:A:638:HOH:O	1:B:302:ARG:NH2	2.47	0.47
1:B:180:PRO:HG3	1:B:263:ASP:OD2	2.15	0.46
1:A:599:GLN:O	1:A:600:GLY:C	2.53	0.46
1:B:227:GLY:HA3	1:B:233:THR:HG21	1.97	0.46
1:B:45:ILE:HG12	1:B:46:ALA:H	1.80	0.46
1:B:45:ILE:HG12	1:B:46:ALA:N	2.30	0.46
1:B:145:PRO:HD2	1:B:355:VAL:O	2.15	0.46
1:A:342:ASP:OD2	1:A:402:HIS:CD2	2.66	0.46
1:B:274:VAL:HA	1:B:282:LEU:O	2.16	0.46
1:A:3:ARG:NH1	1:A:335:GLU:HG3	2.30	0.46
1:B:204:TRP:CD1	1:B:205:GLN:N	2.84	0.46
1:B:243:GLN:HA	1:B:243:GLN:NE2	2.30	0.46
1:A:15:LEU:O	1:A:16:ASP:C	2.52	0.46
1:B:205:GLN:HG3	1:B:254:VAL:HG11	1.98	0.46
1:A:400:LYS:H	1:A:400:LYS:HD2	1.80	0.46
1:B:520:MET:O	1:B:521:TRP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASP:OD1	1:A:403:PRO:HD2	2.16	0.46
1:A:190:VAL:HB	1:A:202:VAL:HB	1.98	0.46
1:A:198:ASN:O	1:A:199:HIS:HB2	2.15	0.46
1:B:547:GLN:NE2	2:B:651:HOH:O	2.49	0.46
1:A:93:HIS:CE1	1:A:138:LEU:HD21	2.51	0.45
1:A:205:GLN:N	1:A:205:GLN:HE21	2.14	0.45
1:A:311:MET:O	1:A:315:HIS:HD2	1.98	0.45
1:B:88:PHE:O	1:B:113:PRO:HA	2.16	0.45
1:B:213:SER:O	1:B:227:GLY:O	2.34	0.45
1:B:282:LEU:CA	1:B:286:LYS:HE3	2.43	0.45
1:B:1:MET:CE	1:B:87:ARG:HH12	2.29	0.45
1:A:105:MET:HE1	1:A:114:PHE:O	2.17	0.45
1:A:65:GLY:H	1:A:136:ASN:ND2	2.15	0.45
1:A:40:GLN:HG2	2:A:801:HOH:O	2.16	0.45
1:B:98:TRP:CH2	1:B:133:CYS:HB2	2.51	0.45
1:B:199:HIS:ND1	1:B:200:ALA:N	2.50	0.45
1:A:240:HIS:N	2:A:697:HOH:O	2.47	0.45
1:B:182:THR:O	1:B:182:THR:CG2	2.64	0.45
1:B:291:THR:HG21	1:B:591:MET:CE	2.47	0.45
1:B:423:GLU:OE1	1:B:424:TYR:N	2.50	0.45
1:B:566:ASN:ND2	1:B:568:LYS:NZ	2.64	0.45
1:A:274:VAL:HG11	1:A:406:VAL:O	2.17	0.45
1:A:419:GLN:HE21	1:A:419:GLN:HA	1.82	0.45
1:A:546:GLU:OE2	1:A:587:ARG:HD3	2.17	0.45
1:B:102:GLN:HG2	1:B:121:TYR:CD1	2.52	0.45
1:B:529:TRP:CZ2	1:B:533:TYR:HE1	2.35	0.45
1:A:185:ASP:OD1	1:A:185:ASP:N	2.50	0.45
1:A:598:GLN:CD	1:A:598:GLN:N	2.69	0.45
1:B:50:SER:OG	1:B:303:GLY:HA3	2.17	0.45
1:B:276:VAL:HG13	1:B:499:PRO:HG2	1.97	0.45
1:A:299:ALA:HB2	1:A:310:LEU:HD11	1.98	0.44
1:A:140:TRP:CB	1:A:379:ALA:O	2.64	0.44
1:A:430:GLU:HG2	2:A:632:HOH:O	2.17	0.44
1:A:472:TYR:CD1	1:A:472:TYR:C	2.91	0.44
1:B:136:ASN:HD22	1:B:136:ASN:H	1.65	0.44
1:B:295:ARG:O	1:B:329:SER:OG	2.28	0.44
1:A:14:LYS:NZ	1:A:14:LYS:HB3	2.33	0.44
1:A:78:GLY:HA3	1:B:78:GLY:HA3	1.99	0.44
1:A:147:MET:O	1:A:159:SER:HB3	2.18	0.44
1:A:3:ARG:NH2	2:A:820:HOH:O	2.43	0.44
1:A:183:TRP:CD1	1:A:183:TRP:C	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLY:HA3	1:A:325:SER:O	2.17	0.44
1:B:50:SER:CB	1:B:303:GLY:HA3	2.47	0.44
1:B:493:GLN:O	1:B:497:HIS:N	2.40	0.44
1:A:203:ASP:CG	1:A:233:THR:HB	2.37	0.44
1:A:242:TRP:CZ2	1:A:345:GLY:HA2	2.53	0.44
1:A:432:THR:OG1	1:A:441:ILE:HD12	2.17	0.44
1:B:9:THR:HA	2:B:697:HOH:O	2.17	0.44
1:B:93:HIS:H	1:B:110:GLY:HA2	1.79	0.44
1:B:561:LEU:HD22	1:B:566:ASN:HD21	1.82	0.44
1:A:227:GLY:HA3	1:A:233:THR:CG2	2.47	0.44
1:B:139:ASN:H	1:B:142:THR:HB	1.83	0.44
1:A:140:TRP:CG	1:A:379:ALA:O	2.71	0.44
1:B:415:ASP:OD2	1:B:417:ARG:NH2	2.51	0.44
1:B:533:TYR:HD2	1:B:537:PHE:CZ	2.35	0.44
1:A:330:HIS:O	1:A:353:ALA:HA	2.18	0.44
1:B:419:GLN:HE21	1:B:419:GLN:HB2	1.62	0.44
1:B:408:TRP:HB2	1:B:441:ILE:HG12	1.99	0.44
1:B:1:MET:HE1	1:B:87:ARG:NH1	2.34	0.43
1:B:243:GLN:HE22	1:B:284:ASN:HD22	1.62	0.43
1:A:47:VAL:HA	1:A:48:PRO:C	2.38	0.43
1:A:14:LYS:HB3	1:A:14:LYS:HZ2	1.81	0.43
1:A:237:VAL:HG12	1:A:238:ASN:H	1.83	0.43
1:A:198:ASN:OD1	1:A:198:ASN:N	2.51	0.43
1:A:243:GLN:HA	1:A:243:GLN:NE2	2.22	0.43
1:B:426:ALA:HA	1:B:459:LEU:HD13	1.99	0.43
1:A:385:GLN:HE22	1:A:427:PRO:HG2	1.83	0.43
1:B:19:TRP:CE2	1:B:71:ARG:HD2	2.53	0.43
1:B:212:VAL:HG23	1:B:214:VAL:HG23	2.00	0.43
1:A:412:ASN:HD21	1:A:466:ASN:ND2	2.12	0.43
1:B:302:ARG:CZ	1:B:302:ARG:HB3	2.49	0.43
1:B:372:LYS:HA	1:B:372:LYS:HD3	1.78	0.43
1:B:471:TRP:CG	1:B:507:VAL:HG12	2.53	0.43
1:B:529:TRP:CE2	1:B:533:TYR:HE1	2.36	0.43
1:A:195:GLN:C	1:A:197:CYS:H	2.22	0.43
1:B:514:HIS:HA	1:B:524:GLU:OE2	2.19	0.43
1:B:328:THR:HG1	1:B:351:GLU:H	1.66	0.43
1:B:357:PHE:HB2	2:B:632:HOH:O	2.18	0.43
1:B:471:TRP:HE3	1:B:520:MET:HE1	1.83	0.43
1:A:107:HIS:CE1	1:A:394:GLU:OE1	2.69	0.43
1:B:295:ARG:HB2	1:B:333:TYR:OH	2.19	0.43
1:B:464:CYS:HA	1:B:501:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:C	1:A:9:THR:H	2.22	0.42
1:A:52:ASN:HB3	1:A:61:ARG:HG3	2.00	0.42
1:A:105:MET:CE	1:A:115:GLU:CA	2.95	0.42
1:A:586:LYS:HE3	1:A:586:LYS:HB2	1.67	0.42
1:B:160:TYR:OH	1:B:557:SER:HB3	2.19	0.42
1:B:194:ALA:CB	1:B:199:HIS:CD2	3.02	0.42
1:B:526:GLN:NE2	2:B:605:HOH:O	2.51	0.42
1:A:64:ALA:HA	1:A:136:ASN:HD21	1.84	0.42
1:B:451:ALA:HB1	1:B:495:LYS:HD2	2.02	0.42
1:B:556:THR:OG1	1:B:562:ARG:CG	2.65	0.42
1:A:8:PRO:HD3	1:B:74:PHE:CE2	2.54	0.42
1:A:222:GLN:NE2	2:A:705:HOH:O	2.52	0.42
1:A:519:ASP:O	1:A:525:TYR:HB2	2.20	0.42
1:B:1:MET:HE1	1:B:115:GLU:CD	2.40	0.42
1:A:507:VAL:CG2	1:A:529:TRP:CD1	3.01	0.42
1:B:413:GLU:HA	1:B:446:VAL:HG22	2.02	0.42
1:A:17:GLY:O	1:A:45:ILE:O	2.38	0.42
1:A:45:ILE:HG13	1:A:55:PHE:CZ	2.54	0.42
1:A:183:TRP:HB3	1:A:263:ASP:HB3	2.02	0.42
1:B:99:VAL:O	1:B:100:ASN:C	2.58	0.42
1:A:269:VAL:HA	2:A:829:HOH:O	2.20	0.42
1:A:311:MET:CE	1:A:340:TRP:CB	2.95	0.42
1:B:263:ASP:CG	2:B:658:HOH:O	2.43	0.42
1:B:282:LEU:HB3	1:B:286:LYS:HZ3	1.85	0.42
1:B:285:HIS:CA	1:B:286:LYS:HZ3	2.32	0.42
1:B:327:ARG:HA	1:B:349:ILE:O	2.19	0.42
1:A:145:PRO:HD2	1:A:355:VAL:O	2.19	0.42
1:A:243:GLN:HE22	1:A:284:ASN:HD22	1.66	0.42
1:A:563:VAL:HG23	1:A:567:LYS:HG2	2.01	0.42
1:B:233:THR:HG22	1:B:234:LEU:H	1.85	0.42
1:B:93:HIS:HB2	1:B:135:ASN:O	2.20	0.41
1:B:519:ASP:OD1	1:B:519:ASP:N	2.45	0.41
1:B:543:VAL:O	1:B:596:LYS:NZ	2.46	0.41
1:A:214:VAL:HG13	1:A:252:LEU:HD11	2.02	0.41
1:B:198:ASN:OD1	1:B:237:VAL:O	2.37	0.41
1:B:451:ALA:HB3	2:B:619:HOH:O	2.20	0.41
1:B:469:TYR:OH	2:B:645:HOH:O	2.20	0.41
1:A:238:ASN:OD1	1:A:238:ASN:N	2.54	0.41
1:B:217:ARG:HG2	1:B:221:GLN:HA	2.02	0.41
1:A:-1:SER:N	2:A:687:HOH:O	2.53	0.41
1:B:105:MET:HE3	1:B:115:GLU:CA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:N	1:B:286:LYS:NZ	2.64	0.41
1:B:426:ALA:HB3	1:B:427:PRO:HD3	2.02	0.41
1:A:79:TRP:HZ3	1:A:176:LEU:HD13	1.86	0.41
1:A:199:HIS:CD2	1:A:200:ALA:N	2.81	0.41
1:B:274:VAL:HG23	1:B:438:THR:O	2.21	0.41
1:A:12:ILE:HG22	1:A:79:TRP:CH2	2.56	0.41
1:A:374:LEU:HD12	1:A:375:TYR:CE2	2.56	0.41
1:B:373:GLU:HB3	1:B:376:SER:HB3	2.03	0.41
1:B:467:ARG:HB3	1:B:533:TYR:OH	2.21	0.41
1:A:167:TYR:HB2	1:A:304:LYS:HG3	2.02	0.41
1:B:205:GLN:NE2	1:B:212:VAL:CG1	2.83	0.41
1:A:83:ARG:HH22	1:A:184:VAL:HG11	1.84	0.41
1:A:180:PRO:HD3	2:A:615:HOH:O	2.20	0.41
1:A:203:ASP:OD2	1:A:233:THR:N	2.48	0.41
1:A:237:VAL:C	1:A:238:ASN:OD1	2.59	0.41
1:B:596:LYS:HD3	2:B:679:HOH:O	2.20	0.41
1:A:9:THR:HA	2:A:615:HOH:O	2.21	0.41
1:B:98:TRP:HH2	1:B:133:CYS:HB2	1.86	0.41
1:A:413:GLU:CB	1:A:446:VAL:HG13	2.51	0.40
1:B:64:ALA:HA	1:B:136:ASN:HD21	1.86	0.40
1:B:183:TRP:CD1	1:B:184:VAL:N	2.89	0.40
1:B:249:LEU:HD13	1:B:268:ARG:HE	1.86	0.40
1:B:583:LEU:HD23	1:B:583:LEU:C	2.42	0.40
1:B:566:ASN:ND2	1:B:568:LYS:HZ1	2.20	0.40
1:B:19:TRP:CD1	1:B:47:VAL:CG1	3.04	0.40
1:B:192:HIS:CD2	1:B:192:HIS:H	2.39	0.40
1:B:216:LEU:HG	1:B:217:ARG:H	1.86	0.40
1:B:278:GLY:O	1:B:499:PRO:HD3	2.21	0.40
1:B:460:PHE:O	1:B:498:GLN:NE2	2.54	0.40
1:B:19:TRP:CD1	1:B:19:TRP:N	2.89	0.40
1:B:356:GLY:C	1:B:358:ASN:H	2.24	0.40
1:A:15:LEU:HD13	1:A:173:SER:OG	2.21	0.40
1:A:17:GLY:O	1:A:46:ALA:HA	2.22	0.40
1:A:83:ARG:HB3	1:A:179:THR:O	2.22	0.40
1:A:111:TYR:HB2	1:A:332:PRO:HD2	2.03	0.40
1:B:1:MET:HE2	1:B:87:ARG:HH12	1.87	0.40
1:B:83:ARG:NH2	1:B:184:VAL:HG13	2.37	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	593/605 (98%)	549 (93%)	35 (6%)	9 (2%)	10	18
1	B	592/605 (98%)	544 (92%)	41 (7%)	7 (1%)	13	24
All	All	1185/1210 (98%)	1093 (92%)	76 (6%)	16 (1%)	11	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	239	PRO
1	B	7	THR
1	B	198	ASN
1	A	600	GLY
1	B	93	HIS
1	A	124	ALA
1	A	550	ASN
1	A	198	ASN
1	B	144	PRO
1	B	357	PHE
1	A	144	PRO
1	B	8	PRO
1	B	239	PRO
1	A	229	GLY
1	A	238	ASN

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	506/513 (99%)	449 (89%)	57 (11%)	6 11
1	B	507/513 (99%)	446 (88%)	61 (12%)	5 9
All	All	1013/1026 (99%)	895 (88%)	118 (12%)	5 10

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	THR
1	A	9	THR
1	A	13	LYS
1	A	15	LEU
1	A	18	LEU
1	A	25	ARG
1	A	47	VAL
1	A	71	ARG
1	A	85	VAL
1	A	99	VAL
1	A	122	VAL
1	A	136	ASN
1	A	148	VAL
1	A	152	GLU
1	A	174	VAL
1	A	176	LEU
1	A	196	ASP
1	A	197	CYS
1	A	203	ASP
1	A	204	TRP
1	A	205	GLN
1	A	209	ASN
1	A	212	VAL
1	A	214	VAL
1	A	216	LEU
1	A	230	THR
1	A	234	LEU
1	A	243	GLN
1	A	258	SER
1	A	272	ARG
1	A	347	VAL
1	A	351	GLU
1	A	355	VAL
1	A	374	LEU

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Mol	Chain	Res	Type
1	A	378	GLU
1	A	383	GLU
1	A	400	LYS
1	A	423	GLU
1	A	432	THR
1	A	446	VAL
1	A	456	ILE
1	A	462	VAL
1	A	467	ARG
1	A	472	TYR
1	A	474	GLN
1	A	483	LYS
1	A	507	VAL
1	A	518	THR
1	A	521	TRP
1	A	530	LEU
1	A	536	VAL
1	A	557	SER
1	A	558	GLN
1	A	562	ARG
1	A	598	GLN
1	A	599	GLN
1	B	7	THR
1	B	11	GLU
1	B	13	LYS
1	B	14	LYS
1	B	15	LEU
1	B	18	LEU
1	B	25	ARG
1	B	47	VAL
1	B	71	ARG
1	B	77	LYS
1	B	82	GLN
1	B	85	VAL
1	B	96	LYS
1	B	99	VAL
1	B	103	GLU
1	B	121	TYR
1	B	136	ASN
1	B	148	VAL
1	B	152	GLU
1	B	156	LYS

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Mol	Chain	Res	Type
1	B	163	ASP
1	B	175	MET
1	B	183	TRP
1	B	185	ASP
1	B	186	ASP
1	B	193	VAL
1	B	195	GLN
1	B	203	ASP
1	B	205	GLN
1	B	206	VAL
1	B	207	VAL
1	B	212	VAL
1	B	234	LEU
1	B	235	GLN
1	B	263	ASP
1	B	267	LEU
1	B	272	ARG
1	B	286	LYS
1	B	298	ASP
1	B	302	ARG
1	B	310	LEU
1	B	329	SER
1	B	347	VAL
1	B	355	VAL
1	B	361	LEU
1	B	372	LYS
1	B	374	LEU
1	B	398	ARG
1	B	400	LYS
1	B	410	ILE
1	B	419	GLN
1	B	438	THR
1	B	462	VAL
1	B	474	GLN
1	B	503	THR
1	B	518	THR
1	B	521	TRP
1	B	531	ASP
1	B	532	MET
1	B	558	GLN
1	B	560	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	66	ASN
1	A	107	HIS
1	A	108	GLN
1	A	135	ASN
1	A	136	ASN
1	A	199	HIS
1	A	209	ASN
1	A	228	GLN
1	A	243	GLN
1	A	313	HIS
1	A	315	HIS
1	A	330	HIS
1	A	385	GLN
1	A	390	GLN
1	A	402	HIS
1	A	412	ASN
1	A	419	GLN
1	A	493	GLN
1	A	514	HIS
1	A	547	GLN
1	A	550	ASN
1	A	592	ASN
1	B	0	HIS
1	B	52	ASN
1	B	82	GLN
1	B	108	GLN
1	B	135	ASN
1	B	136	ASN
1	B	162	HIS
1	B	221	GLN
1	B	222	GLN
1	B	238	ASN
1	B	243	GLN
1	B	280	GLN
1	B	315	HIS
1	B	330	HIS
1	B	388	HIS
1	B	390	GLN
1	B	412	ASN
1	B	419	GLN
1	B	493	GLN

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Mol	Chain	Res	Type
1	B	498	GLN
1	B	514	HIS
1	B	526	GLN
1	B	547	GLN
1	B	566	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	597/605 (98%)	0.28	37 (6%) 20 21	18, 52, 114, 147	0
1	B	596/605 (98%)	0.73	87 (14%) 2 2	27, 93, 178, 229	0
All	All	1193/1210 (98%)	0.50	124 (10%) 6 6	18, 74, 153, 229	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	15.3
1	A	230	THR	9.6
1	B	229	GLY	9.3
1	B	207	VAL	9.0
1	B	208	ALA	8.9
1	A	229	GLY	8.1
1	B	204	TRP	6.1
1	B	282	LEU	5.9
1	A	560	ILE	5.7
1	B	283	ILE	5.6
1	B	230	THR	5.6
1	A	209	ASN	5.4
1	B	259	GLN	5.4
1	B	288	PHE	5.3
1	B	205	GLN	5.2
1	B	545	GLY	5.0
1	A	561	LEU	4.8
1	A	256	ALA	4.8
1	A	183	TRP	4.7
1	B	287	PRO	4.7
1	B	256	ALA	4.4
1	B	598	GLN	4.3
1	B	560	ILE	4.2
1	B	17	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	561	LEU	4.2
1	B	289	TYR	4.2
1	B	209	ASN	4.1
1	B	563	VAL	4.1
1	B	84	ILE	4.1
1	B	1	MET	4.1
1	A	259	GLN	4.1
1	B	196	ASP	4.0
1	B	253	CYS	4.0
1	B	182	THR	3.9
1	A	257	LYS	3.8
1	B	562	ARG	3.8
1	B	152	GLU	3.7
1	B	175	MET	3.7
1	B	565	GLY	3.6
1	B	258	SER	3.5
1	B	206	VAL	3.5
1	A	37	SER	3.5
1	B	337	MET	3.5
1	B	544	VAL	3.5
1	B	262	CYS	3.4
1	B	430	GLU	3.4
1	B	260	THR	3.3
1	B	290	PHE	3.3
1	B	242	TRP	3.3
1	A	239	PRO	3.3
1	B	311	MET	3.2
1	B	419	GLN	3.2
1	B	261	GLU	3.2
1	B	18	LEU	3.2
1	B	214	VAL	3.2
1	A	562	ARG	3.2
1	B	257	LYS	3.2
1	B	105	MET	3.2
1	A	182	THR	3.2
1	A	318	MET	3.1
1	A	208	ALA	3.1
1	B	240	HIS	3.1
1	A	198	ASN	3.1
1	B	153	ASN	3.0
1	A	563	VAL	3.0
1	A	337	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	116	ALA	2.9
1	B	252	LEU	2.9
1	B	361	LEU	2.9
1	A	311	MET	2.8
1	A	260	THR	2.8
1	B	600	GLY	2.8
1	B	236	VAL	2.8
1	A	516	MET	2.8
1	B	255	THR	2.8
1	A	565	GLY	2.8
1	B	537	PHE	2.8
1	A	197	CYS	2.7
1	B	212	VAL	2.7
1	B	67	VAL	2.7
1	B	375	TYR	2.7
1	B	211	ASP	2.6
1	B	425	PHE	2.6
1	B	213	SER	2.6
1	B	564	GLY	2.6
1	A	1	MET	2.6
1	B	468	TYR	2.6
1	B	248	TYR	2.5
1	A	131	THR	2.5
1	B	379	ALA	2.5
1	B	540	VAL	2.5
1	B	597	PRO	2.5
1	B	447	MET	2.5
1	B	489	LEU	2.4
1	B	303	GLY	2.4
1	A	211	ASP	2.4
1	A	175	MET	2.4
1	A	184	VAL	2.4
1	B	357	PHE	2.4
1	B	542	ALA	2.4
1	B	423	GLU	2.4
1	B	463	LEU	2.4
1	A	98	TRP	2.4
1	B	15	LEU	2.4
1	B	228	GLN	2.3
1	A	214	VAL	2.3
1	B	378	GLU	2.3
1	B	264	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	483	LYS	2.3
1	A	34	TRP	2.3
1	A	258	SER	2.3
1	B	594	GLY	2.2
1	A	218	ASP	2.2
1	B	254	VAL	2.2
1	B	123	ILE	2.2
1	B	241	LEU	2.1
1	B	424	TYR	2.1
1	A	40	GLN	2.1
1	B	500	ILE	2.1
1	B	231	SER	2.1
1	B	318	MET	2.1
1	B	280	GLN	2.1
1	A	199	HIS	2.0
1	B	362	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.