Full wwPDB X-ray Structure Validation Report (i)

Sep 30, 2021 – 11:42 AM EDT

PDB ID	:	3MF0
Title	:	Crystal structure of PDE5A GAF domain (89-518)
Authors	:	Wang, H.; Robinson, H.; Ke, H.
Deposited on	:	2010-04-01
Resolution	:	3.10 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 following versions of software and data (see references (1)) were used in the production of this report:

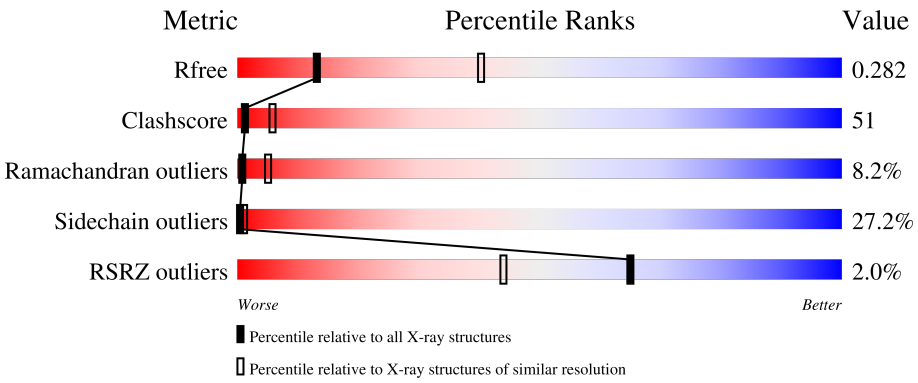
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	432	2% 30% 36% 19% • 12%
1	B	432	2% 27% 35% 22% • 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5921 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 cGMP-specific 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	2994	1894	504	576	20	0	0	0
1	B	369	2927	1852	494	561	20	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

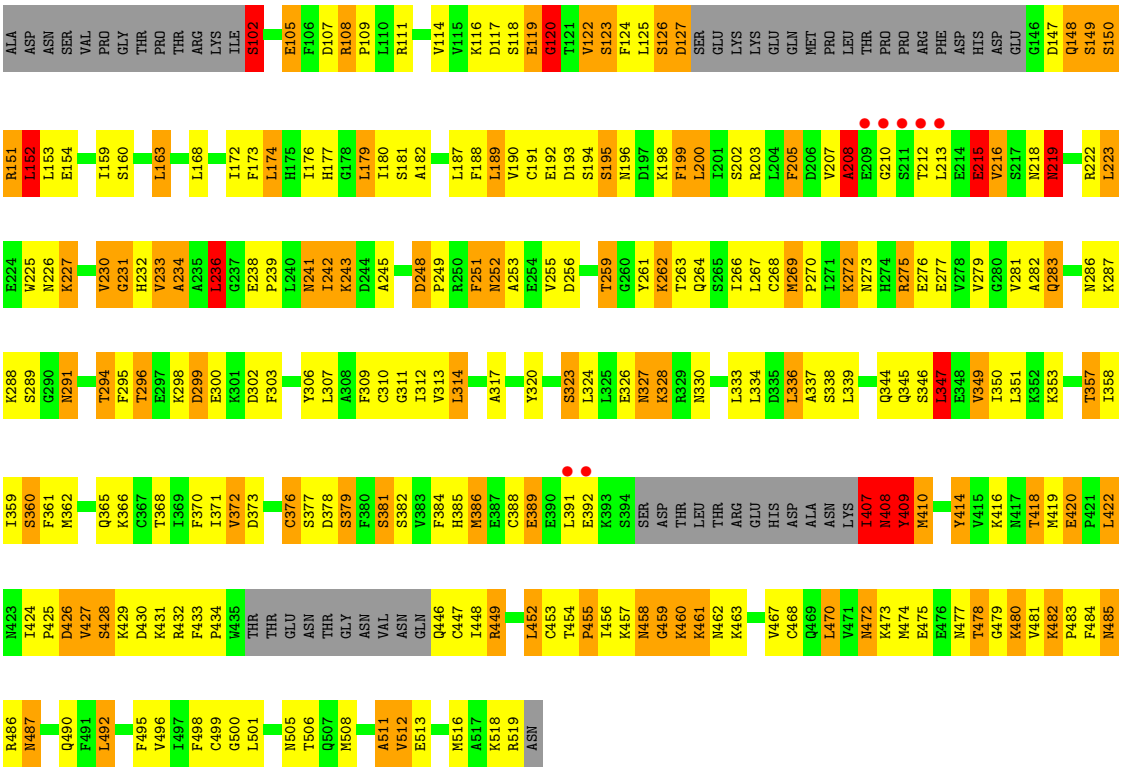
Chain	Residue	Modelled	Actual	Comment	Reference
A	149	SER	CYS	engineered mutation	UNP O76074
A	519	ARG	-	expression tag	UNP O76074
A	520	ASN	-	expression tag	UNP O76074
B	149	SER	CYS	engineered mutation	UNP O76074
B	519	ARG	-	expression tag	UNP O76074
B	520	ASN	-	expression tag	UNP O76074

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.

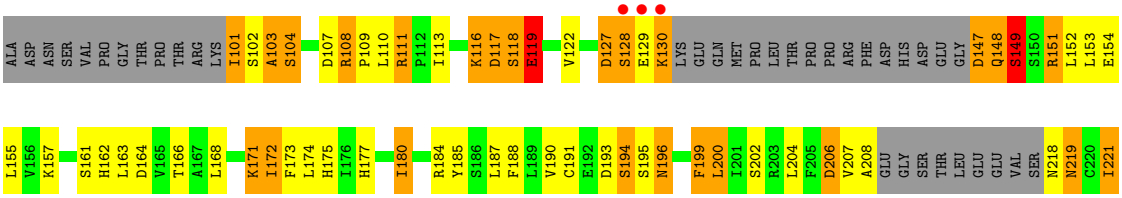
- Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase

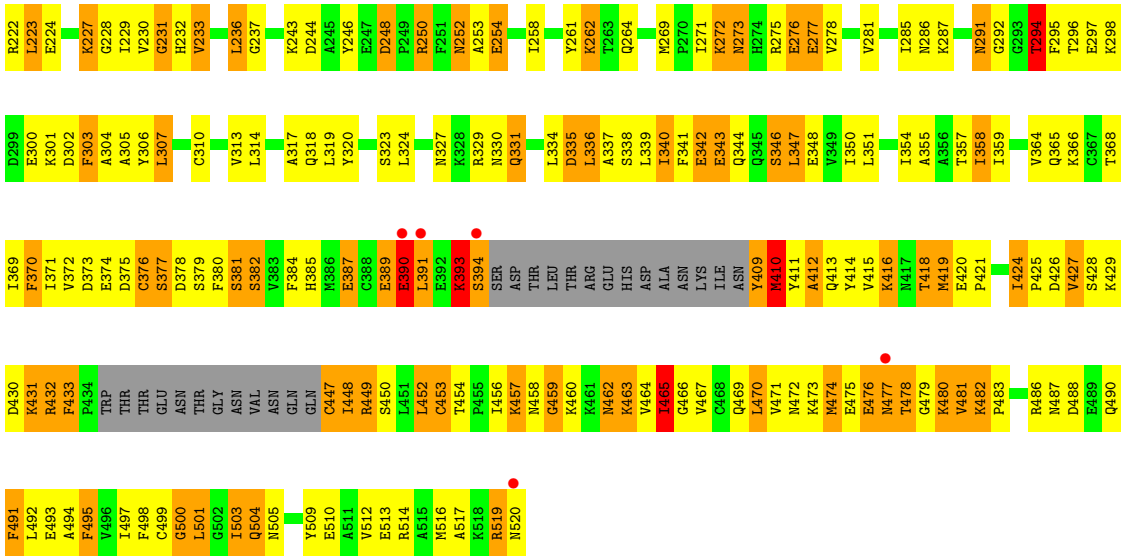
Chain A: 2% 30% 36% 19% • 12%



- Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase

Chain B: 2% 27% 35% 22% • 15%




R222 L223 E224 K227 G228 I229 V230 G231 H232 V233 L236 G237 K243 D244 A245 Y246 E247 D248 P249 R250 F251 N252 A253 E254 I258 Y261 K262 T263 Q264 M269 P270 I271 K272 N273 H274 R275 E276 E277 V278 V281 I285 N286 K287 N291 G292 G293 T294 F295 T296 E297 K298
D299 E300 K301 D302 F303 A304 A305 Y306 L307 C310 V313 L314 A317 Q318 L319 Y320 S323 L324 N327 K328 R329 N330 Q331 L334 D335 L336 A337 S338 L339 I340 F341 E342 E343 Q344 Q345 S346 L347 E348 V349 I350 L351 I354 A355 A356 T357 I358 I359 V364 Q365 K366 C367 T368
I369 F370 I371 V372 D373 E374 D375 C376 S377 D378 S379 F380 S381 S382 V383 F384 H385 M386 E387 C388 E389 E390 L391 E392 K393 S394 SER ASP THR LEU THR ARG GLU HIS ASP ALA ASN LYS ILE ASN Y409 M410 Y411 A412 Q413 Y414 V415 K416 N417 T418 M419 E420 P421 I424 P425 D426 V427 S428 K429
D430 K431 R432 F433 P434 TRP THR THR GLU ASN THR GLY ASN VAL ASN GLN GLN C447 I448 R449 S450 L451 L452 C453 T454 P455 I456 K457 N458 G459 K460 K461 N462 K463 V464 I465 G466 V467 C468 Q469 L470 V471 N472 K473 M474 E475 E476 N477 T478 G479 K480 V481 K482 P483 R486 N487 D488 E489 Q490
F491 L492 E493 A494 F495 V496 I497 F498 C499 G500 L501 G502 I503 Q504 N505 Y509 E510 A511 V512 E513 R514 A515 M516 A517 K518 R519 N520

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.53Å 144.53Å 135.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.71 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.10) 99.6 (29.71-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.289 0.223 , 0.282	Depositor DCC
R_{free} test set	1507 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	95.4	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5921	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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	0.55	0/3041	0.67	2/4096 (0.0%)
1	B	0.54	0/2971	0.67	2/3996 (0.1%)
All	All	0.54	0/6012	0.67	4/8092 (0.0%)

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	25
1	B	0	14
All	All	0	39

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	336	LEU	CB-CG-CD2	6.61	122.23	111.00
1	B	319	LEU	CA-CB-CG	-5.98	101.54	115.30
1	A	236	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	223	LEU	CA-CB-CG	-5.00	103.80	115.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	SER	Peptide
1	A	118	SER	Peptide
1	A	120	GLY	Peptide
1	A	125	LEU	Peptide
1	A	148	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	188	PHE	Mainchain
1	A	192	GLU	Mainchain
1	A	208	ALA	Peptide
1	A	210	GLY	Peptide
1	A	215	GLU	Peptide
1	A	218	ASN	Peptide
1	A	219	ASN	Peptide
1	A	236	LEU	Mainchain
1	A	251	PHE	Sidechain
1	A	270	PRO	Mainchain
1	A	388	CYS	Peptide
1	A	389	GLU	Peptide
1	A	391	LEU	Peptide
1	A	407	ILE	Peptide
1	A	408	ASN	Mainchain
1	A	447	CYS	Peptide
1	A	459	GLY	Peptide
1	A	460	LYS	Peptide
1	A	477	ASN	Peptide
1	A	518	LYS	Peptide
1	B	118	SER	Peptide
1	B	128	SER	Peptide
1	B	147	ASP	Peptide
1	B	206	ASP	Peptide
1	B	224	GLU	Peptide
1	B	228	GLY	Peptide
1	B	304	ALA	Peptide
1	B	376	CYS	Peptide
1	B	382	SER	Peptide
1	B	387	GLU	Peptide
1	B	393	LYS	Peptide
1	B	410	MET	Peptide
1	B	481	VAL	Peptide
1	B	491	PHE	Sidechain

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	2994	0	2984	270	0
1	B	2927	0	2928	357	0
All	All	5921	0	5912	600	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 51.

All (600) 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:478:THR:CG2	1:B:480:LYS:H	1.23	1.47
1:B:478:THR:HG22	1:B:480:LYS:N	1.31	1.41
1:B:453:CYS:SG	1:B:469:GLN:HB3	1.79	1.23
1:A:452:LEU:HB2	1:A:484:PHE:CD1	1.74	1.21
1:B:102:SER:O	1:B:104:SER:N	1.74	1.20
1:A:478:THR:HG22	1:A:480:LYS:N	1.54	1.20
1:A:478:THR:CG2	1:A:480:LYS:H	1.57	1.18
1:B:101:ILE:HD12	1:B:101:ILE:N	1.60	1.15
1:A:205:PHE:HD1	1:A:205:PHE:O	1.31	1.13
1:B:491:PHE:CZ	1:B:495:PHE:HD1	1.67	1.12
1:A:478:THR:HG21	1:A:480:LYS:HB2	1.20	1.09
1:B:147:ASP:HB2	1:B:149:SER:HB2	1.33	1.08
1:B:478:THR:HG21	1:B:480:LYS:HB3	1.22	1.08
1:A:414:TYR:CD1	1:A:433:PHE:HZ	1.72	1.06
1:B:491:PHE:CZ	1:B:495:PHE:CD1	2.43	1.05
1:B:110:LEU:HD12	1:B:329:ARG:NH1	1.72	1.04
1:B:448:ILE:HG22	1:B:448:ILE:O	1.51	1.03
1:A:205:PHE:O	1:A:205:PHE:CD1	2.13	1.01
1:A:108:ARG:HB2	1:A:109:PRO:HD2	1.42	1.01
1:A:245:ALA:HB1	1:A:251:PHE:CD2	1.96	1.00
1:B:250:ARG:HG2	1:B:250:ARG:HH11	1.25	0.99
1:B:269:MET:HE3	1:B:303:PHE:HB3	1.42	0.99
1:B:351:LEU:HD22	1:B:369:ILE:HG21	1.41	0.98
1:B:336:LEU:HB2	1:B:495:PHE:CE1	1.99	0.97
1:B:116:LYS:NZ	1:B:493:GLU:OE2	1.97	0.97
1:B:428:SER:O	1:B:429:LYS:HG2	1.64	0.97
1:B:250:ARG:HH11	1:B:250:ARG:CG	1.78	0.96
1:B:199:PHE:HD1	1:B:199:PHE:H	1.00	0.96
1:A:414:TYR:CD1	1:A:433:PHE:CZ	2.54	0.95
1:A:478:THR:HG21	1:A:480:LYS:CB	1.95	0.95
1:B:448:ILE:O	1:B:448:ILE:CG2	2.14	0.94
1:A:227:LYS:O	1:A:231:GLY:HA3	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:O	1:B:380:PHE:HD2	1.51	0.93
1:A:512:VAL:HG21	1:B:509:TYR:CE1	2.02	0.93
1:A:414:TYR:HD1	1:A:433:PHE:CZ	1.85	0.93
1:B:294:THR:HG23	1:B:295:PHE:N	1.82	0.93
1:B:410:MET:O	1:B:413:GLN:HB2	1.68	0.92
1:A:470:LEU:HD21	1:A:492:LEU:HD11	1.51	0.92
1:B:458:ASN:HB2	1:B:465:ILE:HD11	1.50	0.91
1:B:199:PHE:HD1	1:B:199:PHE:N	1.67	0.91
1:B:177:HIS:HD2	1:B:185:TYR:CD2	1.90	0.90
1:B:409:TYR:HD1	1:B:409:TYR:O	1.53	0.90
1:B:287:LYS:HD3	1:B:294:THR:O	1.70	0.90
1:B:221:ILE:CG2	1:B:223:LEU:HD21	2.01	0.90
1:B:368:THR:HG23	1:B:385:HIS:HB2	1.52	0.90
1:B:453:CYS:SG	1:B:469:GLN:CB	2.58	0.90
1:A:251:PHE:HE1	1:A:253:ALA:HA	1.35	0.90
1:B:264:GLN:HB3	1:B:286:ASN:OD1	1.72	0.89
1:B:336:LEU:CB	1:B:495:PHE:CZ	2.55	0.89
1:B:428:SER:O	1:B:429:LYS:CG	2.19	0.89
1:B:336:LEU:HB2	1:B:495:PHE:CZ	2.08	0.89
1:A:452:LEU:CB	1:A:484:PHE:CD1	2.55	0.88
1:A:245:ALA:HB1	1:A:251:PHE:HD2	1.34	0.88
1:B:478:THR:CG2	1:B:480:LYS:HB3	2.02	0.88
1:A:222:ARG:O	1:A:222:ARG:HG2	1.73	0.88
1:A:275:ARG:HG3	1:A:275:ARG:HH11	1.37	0.88
1:B:491:PHE:HZ	1:B:495:PHE:CD1	1.86	0.88
1:A:426:ASP:HA	1:A:449:ARG:O	1.73	0.87
1:B:379:SER:O	1:B:380:PHE:CD2	2.28	0.87
1:A:376:CYS:SG	1:A:376:CYS:O	2.33	0.86
1:A:306:TYR:CE2	1:A:310:CYS:SG	2.68	0.86
1:A:153:LEU:HD21	1:B:153:LEU:HG	1.55	0.86
1:B:478:THR:HG21	1:B:480:LYS:CB	2.05	0.86
1:B:473:LYS:HE2	1:B:488:ASP:OD2	1.74	0.86
1:B:336:LEU:CB	1:B:495:PHE:HZ	1.89	0.86
1:A:478:THR:CG2	1:A:480:LYS:HB2	2.06	0.85
1:B:101:ILE:N	1:B:101:ILE:CD1	2.32	0.85
1:B:269:MET:CE	1:B:303:PHE:HB3	2.06	0.85
1:B:177:HIS:CD2	1:B:185:TYR:CD2	2.64	0.84
1:B:109:PRO:O	1:B:110:LEU:HD23	1.77	0.84
1:B:223:LEU:HD23	1:B:223:LEU:N	1.91	0.84
1:B:478:THR:CG2	1:B:480:LYS:N	2.07	0.84
1:B:184:ARG:NH2	1:B:261:TYR:CD1	2.46	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:CYS:O	1:B:449:ARG:N	2.11	0.83
1:B:481:VAL:HG12	1:B:482:LYS:H	1.43	0.83
1:A:422:LEU:HD21	1:A:424:ILE:HD11	1.58	0.83
1:A:163:LEU:HD13	1:A:320:TYR:CG	2.13	0.83
1:A:452:LEU:HB2	1:A:484:PHE:HD1	1.43	0.83
1:B:269:MET:HE1	1:B:300:GLU:O	1.79	0.83
1:B:127:ASP:O	1:B:129:GLU:HB2	1.77	0.83
1:B:450:SER:OG	1:B:472:ASN:HA	1.78	0.82
1:A:422:LEU:CD2	1:A:424:ILE:HD11	2.09	0.82
1:A:485:ASN:C	1:A:485:ASN:HD22	1.79	0.82
1:B:336:LEU:O	1:B:495:PHE:CZ	2.32	0.82
1:A:426:ASP:OD1	1:A:426:ASP:C	2.19	0.81
1:B:454:THR:OG1	1:B:492:LEU:HD23	1.81	0.81
1:B:409:TYR:O	1:B:409:TYR:CD1	2.33	0.81
1:B:476:GLU:O	1:B:477:ASN:HB2	1.78	0.80
1:B:371:ILE:HD12	1:B:371:ILE:N	1.95	0.80
1:A:116:LYS:HG2	1:A:120:GLY:HA3	1.63	0.80
1:B:195:SER:C	1:B:196:ASN:HD22	1.86	0.80
1:B:462:ASN:HD22	1:B:462:ASN:C	1.86	0.79
1:A:353:LYS:O	1:A:357:THR:HB	1.80	0.79
1:B:481:VAL:CG1	1:B:482:LYS:H	1.95	0.79
1:A:454:THR:HG22	1:A:455:PRO:N	1.98	0.79
1:B:222:ARG:C	1:B:223:LEU:HD23	2.04	0.79
1:B:393:LYS:O	1:B:394:SER:HB3	1.83	0.78
1:A:454:THR:HG23	1:A:455:PRO:HD2	1.66	0.77
1:B:373:ASP:HA	1:B:381:SER:OG	1.84	0.77
1:A:267:LEU:O	1:A:283:GLN:HB2	1.85	0.77
1:A:294:THR:HG23	1:A:295:PHE:H	1.48	0.77
1:B:481:VAL:HG12	1:B:482:LYS:N	2.00	0.77
1:B:478:THR:CG2	1:B:480:LYS:CB	2.63	0.76
1:B:453:CYS:HG	1:B:469:GLN:HB3	1.50	0.76
1:A:336:LEU:HD13	1:A:357:THR:CG2	2.16	0.76
1:A:233:VAL:HG21	1:A:268:CYS:SG	2.25	0.75
1:B:200:LEU:HD23	1:B:200:LEU:N	2.00	0.75
1:B:376:CYS:HA	1:B:377:SER:HB2	1.66	0.75
1:B:482:LYS:HG2	1:B:483:PRO:HD2	1.67	0.75
1:A:163:LEU:HD13	1:A:320:TYR:CD2	2.22	0.75
1:B:420:GLU:HB3	1:B:421:PRO:HD2	1.68	0.74
1:B:486:ARG:HG3	1:B:486:ARG:HH11	1.52	0.74
1:A:478:THR:HG22	1:A:480:LYS:H	0.68	0.74
1:A:153:LEU:HD23	1:B:153:LEU:CD2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:THR:CG2	1:A:455:PRO:N	2.51	0.73
1:A:296:THR:HB	1:A:299:ASP:H	1.52	0.73
1:A:251:PHE:CE1	1:A:253:ALA:HA	2.20	0.73
1:A:251:PHE:HE2	1:A:263:THR:HG21	1.53	0.73
1:B:200:LEU:N	1:B:200:LEU:CD2	2.51	0.73
1:B:336:LEU:HB3	1:B:495:PHE:CZ	2.23	0.73
1:B:152:LEU:O	1:B:155:LEU:HB2	1.88	0.73
1:B:347:LEU:HD22	1:B:351:LEU:HD11	1.69	0.73
1:A:243:LYS:HG3	1:A:294:THR:OG1	1.89	0.73
1:A:409:TYR:H	1:A:409:TYR:HD2	1.37	0.73
1:A:200:LEU:N	1:A:200:LEU:CD2	2.52	0.72
1:B:336:LEU:HB2	1:B:495:PHE:HE1	1.50	0.72
1:B:366:LYS:HB2	1:B:471:VAL:CG2	2.20	0.72
1:A:496:VAL:HA	1:A:499:CYS:HB2	1.69	0.72
1:B:414:TYR:O	1:B:418:THR:OG1	2.08	0.72
1:A:430:ASP:OD1	1:A:432:ARG:HB2	1.89	0.72
1:B:269:MET:HG3	1:B:303:PHE:CD1	2.25	0.72
1:A:108:ARG:HB2	1:A:109:PRO:CD	2.18	0.72
1:B:275:ARG:NH1	1:B:277:GLU:CD	2.43	0.72
1:B:221:ILE:CG2	1:B:223:LEU:CD2	2.68	0.71
1:B:452:LEU:HD12	1:B:453:CYS:N	2.06	0.71
1:B:336:LEU:O	1:B:495:PHE:HZ	1.70	0.71
1:B:294:THR:CG2	1:B:295:PHE:N	2.53	0.71
1:B:275:ARG:NH1	1:B:277:GLU:OE1	2.24	0.71
1:B:102:SER:C	1:B:104:SER:H	1.92	0.71
1:A:330:ASN:HD22	1:B:327:ASN:HD21	1.39	0.71
1:B:272:LYS:HG2	1:B:276:GLU:O	1.91	0.71
1:A:287:LYS:HD3	1:A:294:THR:O	1.91	0.71
1:B:117:ASP:O	1:B:119:GLU:N	2.23	0.71
1:A:102:SER:HA	1:A:361:PHE:CD1	2.26	0.70
1:A:294:THR:HG23	1:A:295:PHE:N	2.05	0.70
1:B:163:LEU:HD13	1:B:320:TYR:CG	2.25	0.70
1:A:126:SER:O	1:A:127:ASP:HB2	1.91	0.70
1:A:378:ASP:OD2	1:A:379:SER:HB3	1.92	0.70
1:A:242:ILE:HG13	1:A:266:ILE:HB	1.72	0.70
1:A:306:TYR:C	1:A:306:TYR:CD2	2.64	0.70
1:A:179:LEU:HD13	1:A:180:ILE:HG23	1.72	0.70
1:A:294:THR:CG2	1:A:295:PHE:N	2.54	0.70
1:A:358:ILE:HG23	1:A:362:MET:HG3	1.72	0.70
1:B:294:THR:HG23	1:B:295:PHE:H	1.54	0.70
1:B:342:GLU:HG3	1:B:343:GLU:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:CE	1:A:303:PHE:HB3	2.21	0.70
1:B:250:ARG:CG	1:B:250:ARG:NH1	2.45	0.69
1:B:162:HIS:NE2	1:B:171:LYS:HE2	2.08	0.69
1:B:373:ASP:CB	1:B:379:SER:HB2	2.23	0.69
1:A:222:ARG:O	1:A:222:ARG:CG	2.41	0.69
1:A:368:THR:HG22	1:A:370:PHE:CE1	2.28	0.69
1:A:473:LYS:HB2	1:A:484:PHE:CE2	2.27	0.69
1:B:108:ARG:HB2	1:B:109:PRO:HD2	1.75	0.69
1:B:155:LEU:HD22	1:B:175:HIS:CG	2.28	0.68
1:A:182:ALA:HA	1:A:288:LYS:H	1.59	0.68
1:B:199:PHE:N	1:B:199:PHE:CD1	2.41	0.68
1:A:116:LYS:CG	1:A:120:GLY:HA3	2.23	0.67
1:A:306:TYR:HE2	1:A:310:CYS:SG	2.18	0.67
1:B:102:SER:C	1:B:104:SER:N	2.48	0.67
1:B:370:PHE:C	1:B:371:ILE:HD12	2.15	0.67
1:B:481:VAL:CG1	1:B:482:LYS:N	2.56	0.67
1:B:355:ALA:O	1:B:359:ILE:HG13	1.94	0.67
1:A:275:ARG:HG3	1:A:275:ARG:NH1	2.08	0.66
1:A:349:VAL:HG12	1:A:350:ILE:N	2.09	0.66
1:B:458:ASN:HB3	1:B:465:ILE:CG1	2.26	0.66
1:B:221:ILE:HG21	1:B:223:LEU:HD21	1.77	0.66
1:B:366:LYS:HB2	1:B:471:VAL:HG23	1.76	0.66
1:B:376:CYS:CA	1:B:377:SER:HB2	2.26	0.66
1:B:354:ILE:HD13	1:B:499:CYS:SG	2.36	0.66
1:B:478:THR:HG22	1:B:480:LYS:H	0.50	0.66
1:A:336:LEU:HD13	1:A:357:THR:HG21	1.76	0.65
1:A:485:ASN:C	1:A:485:ASN:ND2	2.50	0.65
1:B:336:LEU:HB3	1:B:495:PHE:HZ	1.57	0.65
1:B:310:CYS:O	1:B:314:LEU:HB2	1.96	0.65
1:A:255:VAL:O	1:A:259:THR:HG23	1.96	0.65
1:A:512:VAL:CG2	1:B:509:TYR:CE1	2.78	0.65
1:A:195:SER:O	1:A:196:ASN:HB2	1.97	0.65
1:B:370:PHE:HD1	1:B:370:PHE:N	1.94	0.65
1:B:223:LEU:N	1:B:223:LEU:CD2	2.61	0.64
1:B:457:LYS:O	1:B:465:ILE:HG13	1.97	0.64
1:B:418:THR:O	1:B:419:MET:HB2	1.96	0.64
1:B:373:ASP:HB2	1:B:379:SER:HB2	1.76	0.64
1:B:462:ASN:HD22	1:B:463:LYS:N	1.95	0.64
1:A:478:THR:CG2	1:A:480:LYS:CB	2.73	0.64
1:B:273:ASN:C	1:B:273:ASN:OD1	2.36	0.63
1:A:418:THR:HG22	1:A:420:GLU:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HG21	1:B:453:CYS:HB3	1.80	0.63
1:B:180:ILE:O	1:B:185:TYR:OH	2.14	0.63
1:B:370:PHE:CD2	1:B:412:ALA:CB	2.81	0.63
1:A:200:LEU:N	1:A:200:LEU:HD22	2.14	0.63
1:A:366:LYS:HD3	1:A:385:HIS:CE1	2.34	0.62
1:B:450:SER:OG	1:B:472:ASN:CA	2.47	0.62
1:B:478:THR:HG22	1:B:479:GLY:N	2.07	0.62
1:A:230:VAL:O	1:A:231:GLY:C	2.37	0.62
1:B:370:PHE:N	1:B:370:PHE:CD1	2.66	0.62
1:B:185:TYR:N	1:B:206:ASP:OD1	2.27	0.62
1:A:243:LYS:CG	1:A:294:THR:OG1	2.47	0.62
1:A:428:SER:O	1:A:429:LYS:HG3	1.99	0.62
1:A:198:LYS:O	1:A:199:PHE:HB3	1.99	0.62
1:B:371:ILE:N	1:B:371:ILE:CD1	2.62	0.62
1:A:505:ASN:ND2	1:B:344:GLN:H	1.97	0.62
1:A:512:VAL:HG21	1:B:509:TYR:CZ	2.35	0.62
1:A:153:LEU:HD23	1:B:153:LEU:HD21	1.82	0.61
1:B:194:SER:OG	1:B:487:ASN:HB2	2.00	0.61
1:B:458:ASN:ND2	1:B:463:LYS:H	1.97	0.61
1:B:258:ILE:HG22	1:B:258:ILE:O	1.99	0.61
1:A:452:LEU:C	1:A:452:LEU:CD2	2.69	0.61
1:B:376:CYS:SG	1:B:377:SER:HB2	2.41	0.61
1:B:472:ASN:HB3	1:B:481:VAL:HG22	1.82	0.61
1:B:173:PHE:HB2	1:B:204:LEU:HD13	1.82	0.61
1:A:256:ASP:OD2	1:A:261:TYR:O	2.19	0.60
1:B:147:ASP:HB2	1:B:149:SER:CB	2.19	0.60
1:B:199:PHE:O	1:B:200:LEU:HD22	2.00	0.60
1:B:190:VAL:HG12	1:B:191:CYS:N	2.15	0.60
1:B:102:SER:O	1:B:103:ALA:C	2.39	0.60
1:B:503:ILE:HG22	1:B:504:GLN:N	2.15	0.60
1:A:241:ASN:HD21	1:A:295:PHE:HB2	1.67	0.60
1:B:291:ASN:H	1:B:291:ASN:ND2	2.00	0.60
1:A:291:ASN:HD22	1:A:291:ASN:N	1.99	0.60
1:B:291:ASN:H	1:B:291:ASN:HD22	1.49	0.60
1:B:108:ARG:HB2	1:B:109:PRO:CD	2.32	0.59
1:A:336:LEU:HD13	1:A:357:THR:HG23	1.83	0.59
1:B:458:ASN:CB	1:B:465:ILE:CG1	2.80	0.59
1:B:366:LYS:O	1:B:470:LEU:HA	2.03	0.59
1:A:336:LEU:CD1	1:A:357:THR:HG23	2.33	0.59
1:B:252:ASN:C	1:B:252:ASN:ND2	2.56	0.59
1:A:264:GLN:N	1:A:286:ASN:OD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HD22	1:B:369:ILE:CG2	2.26	0.59
1:B:262:LYS:HG3	1:B:262:LYS:O	2.03	0.59
1:A:372:VAL:HG22	1:A:416:LYS:HD2	1.84	0.59
1:A:505:ASN:HD21	1:B:344:GLN:H	1.51	0.59
1:B:458:ASN:O	1:B:459:GLY:C	2.42	0.58
1:B:458:ASN:HB2	1:B:465:ILE:CD1	2.30	0.58
1:B:464:VAL:O	1:B:464:VAL:HG12	2.03	0.58
1:B:184:ARG:NH2	1:B:261:TYR:CG	2.71	0.58
1:B:199:PHE:C	1:B:200:LEU:CD2	2.72	0.58
1:B:458:ASN:HB3	1:B:465:ILE:HG13	1.86	0.58
1:B:458:ASN:CB	1:B:465:ILE:HD11	2.27	0.58
1:A:291:ASN:HD22	1:A:291:ASN:H	1.50	0.58
1:B:190:VAL:CG1	1:B:191:CYS:N	2.66	0.58
1:A:408:ASN:O	1:A:410:MET:N	2.36	0.58
1:A:242:ILE:HD12	1:A:248:ASP:OD1	2.04	0.58
1:A:470:LEU:CD2	1:A:492:LEU:HD11	2.30	0.58
1:B:177:HIS:HD2	1:B:185:TYR:CE2	2.21	0.58
1:B:476:GLU:HA	1:B:476:GLU:OE2	2.04	0.58
1:A:359:ILE:HD11	1:A:386:MET:HB3	1.85	0.57
1:A:454:THR:HG23	1:A:455:PRO:CD	2.34	0.57
1:A:418:THR:HG23	1:A:420:GLU:HG3	1.87	0.57
1:B:148:GLN:O	1:B:151:ARG:N	2.37	0.57
1:B:109:PRO:C	1:B:110:LEU:HD23	2.25	0.57
1:B:482:LYS:CG	1:B:483:PRO:HD2	2.33	0.57
1:A:111:ARG:HG3	1:A:326:GLU:OE2	2.04	0.57
1:B:285:ILE:O	1:B:286:ASN:HB2	2.04	0.57
1:B:168:LEU:O	1:B:172:ILE:HG13	2.05	0.57
1:A:264:GLN:HB3	1:A:286:ASN:OD1	2.05	0.57
1:B:113:ILE:HG22	1:B:490:GLN:OE1	2.04	0.57
1:B:221:ILE:HG23	1:B:223:LEU:HD21	1.84	0.57
1:A:163:LEU:HD13	1:A:320:TYR:CB	2.35	0.57
1:A:230:VAL:O	1:A:232:HIS:N	2.37	0.57
1:A:452:LEU:C	1:A:452:LEU:HD22	2.25	0.57
1:A:479:GLY:O	1:A:480:LYS:O	2.23	0.57
1:B:230:VAL:HG23	1:B:231:GLY:N	2.20	0.57
1:B:172:ILE:HG23	1:B:310:CYS:SG	2.45	0.56
1:A:508:MET:O	1:A:511:ALA:HB3	2.05	0.56
1:B:296:THR:C	1:B:298:LYS:H	2.07	0.56
1:A:153:LEU:CD2	1:B:153:LEU:HG	2.31	0.56
1:A:519:ARG:HB2	1:A:519:ARG:NH1	2.20	0.56
1:B:428:SER:O	1:B:429:LYS:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:CG2	1:B:222:ARG:N	2.67	0.56
1:B:354:ILE:O	1:B:358:ILE:HG12	2.06	0.56
1:B:478:THR:CG2	1:B:480:LYS:CA	2.83	0.56
1:A:267:LEU:O	1:A:283:GLN:HA	2.06	0.56
1:B:486:ARG:HG3	1:B:486:ARG:NH1	2.20	0.56
1:A:479:GLY:C	1:A:480:LYS:O	2.44	0.55
1:B:148:GLN:HB3	1:B:151:ARG:HB3	1.88	0.55
1:B:248:ASP:OD2	1:B:250:ARG:HD2	2.06	0.55
1:B:428:SER:C	1:B:429:LYS:CG	2.75	0.55
1:B:462:ASN:C	1:B:462:ASN:ND2	2.59	0.55
1:A:117:ASP:C	1:A:120:GLY:HA2	2.27	0.55
1:B:116:LYS:HD3	1:B:122:VAL:HG12	1.88	0.55
1:B:195:SER:O	1:B:196:ASN:HB2	2.06	0.55
1:A:124:PHE:O	1:B:331:GLN:NE2	2.39	0.55
1:B:368:THR:CG2	1:B:370:PHE:HE1	2.19	0.55
1:A:470:LEU:HD21	1:A:492:LEU:CD1	2.32	0.55
1:B:287:LYS:CD	1:B:294:THR:O	2.51	0.55
1:B:119:GLU:HG3	1:B:119:GLU:O	2.06	0.55
1:A:358:ILE:O	1:A:359:ILE:C	2.44	0.55
1:B:188:PHE:CD2	1:B:202:SER:HB2	2.42	0.55
1:A:163:LEU:CD1	1:A:320:TYR:CG	2.87	0.55
1:B:368:THR:HG22	1:B:370:PHE:CE1	2.42	0.55
1:B:464:VAL:O	1:B:466:GLY:N	2.39	0.55
1:B:491:PHE:C	1:B:491:PHE:CD2	2.79	0.55
1:A:328:LYS:NZ	1:B:129:GLU:HB3	2.21	0.54
1:B:368:THR:CG2	1:B:370:PHE:CE1	2.90	0.54
1:B:370:PHE:CD2	1:B:412:ALA:HB2	2.43	0.54
1:A:346:SER:HB3	1:A:349:VAL:HB	1.88	0.54
1:B:271:ILE:CG1	1:B:307:LEU:HD13	2.37	0.54
1:A:116:LYS:HG2	1:A:120:GLY:CA	2.34	0.54
1:B:419:MET:CE	1:B:464:VAL:HG23	2.37	0.54
1:B:478:THR:HG22	1:B:479:GLY:C	2.20	0.54
1:A:272:LYS:O	1:A:311:GLY:HA3	2.07	0.54
1:B:454:THR:HG1	1:B:492:LEU:HD23	1.69	0.54
1:B:193:ASP:O	1:B:195:SER:N	2.41	0.54
1:A:116:LYS:HG3	1:A:122:VAL:HG23	1.89	0.54
1:B:199:PHE:C	1:B:200:LEU:HD22	2.28	0.54
1:B:424:ILE:HG22	1:B:426:ASP:O	2.07	0.54
1:A:409:TYR:N	1:A:409:TYR:CD2	2.74	0.54
1:B:119:GLU:O	1:B:119:GLU:CG	2.56	0.54
1:A:336:LEU:CD1	1:A:357:THR:CG2	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:THR:C	1:B:298:LYS:N	2.62	0.53
1:A:223:LEU:HD13	1:A:230:VAL:HG22	1.89	0.53
1:B:194:SER:CB	1:B:487:ASN:H	2.21	0.53
1:B:491:PHE:CE2	1:B:495:PHE:HB2	2.44	0.53
1:B:465:ILE:CD1	1:B:504:GLN:HB2	2.38	0.53
1:A:153:LEU:CD2	1:B:153:LEU:CD2	2.85	0.53
1:B:482:LYS:HG2	1:B:483:PRO:CD	2.38	0.53
1:A:296:THR:HB	1:A:299:ASP:N	2.23	0.53
1:B:254:GLU:O	1:B:258:ILE:HG13	2.09	0.53
1:B:336:LEU:CB	1:B:495:PHE:CE1	2.79	0.53
1:A:269:MET:HE1	1:A:300:GLU:O	2.07	0.53
1:A:267:LEU:O	1:A:283:GLN:CB	2.56	0.53
1:B:230:VAL:O	1:B:232:HIS:N	2.42	0.52
1:A:422:LEU:HD23	1:A:424:ILE:HG13	1.91	0.52
1:A:159:ILE:HD12	1:A:313:VAL:HG21	1.89	0.52
1:B:173:PHE:CD2	1:B:204:LEU:HB3	2.44	0.52
1:A:310:CYS:O	1:A:314:LEU:HB2	2.09	0.52
1:A:347:LEU:O	1:A:351:LEU:HG	2.10	0.52
1:B:419:MET:C	1:B:420:GLU:HG2	2.29	0.52
1:B:230:VAL:CG2	1:B:231:GLY:N	2.73	0.52
1:B:517:ALA:HA	1:B:520:ASN:OXT	2.10	0.52
1:A:320:TYR:CE2	1:A:324:LEU:HD11	2.45	0.52
1:B:351:LEU:CD2	1:B:369:ILE:HG21	2.25	0.52
1:B:368:THR:HB	1:B:370:PHE:HE1	1.75	0.52
1:B:168:LEU:O	1:B:172:ILE:CG1	2.57	0.51
1:B:221:ILE:HG23	1:B:223:LEU:CD2	2.39	0.51
1:B:419:MET:HE3	1:B:464:VAL:HG23	1.91	0.51
1:A:119:GLU:O	1:A:120:GLY:C	2.47	0.51
1:A:163:LEU:CD1	1:A:320:TYR:CD2	2.92	0.51
1:A:179:LEU:CD1	1:A:303:PHE:HA	2.40	0.51
1:B:258:ILE:O	1:B:258:ILE:CG2	2.59	0.51
1:B:458:ASN:O	1:B:459:GLY:O	2.28	0.51
1:B:464:VAL:O	1:B:465:ILE:C	2.48	0.51
1:B:188:PHE:N	1:B:281:VAL:O	2.36	0.51
1:B:416:LYS:O	1:B:416:LYS:HE3	2.10	0.51
1:B:148:GLN:HA	1:B:151:ARG:HB3	1.93	0.51
1:B:465:ILE:HD12	1:B:504:GLN:HB2	1.92	0.51
1:B:498:PHE:HA	1:B:501:LEU:HD12	1.93	0.51
1:A:273:ASN:OD1	1:A:277:GLU:HB2	2.10	0.51
1:A:365:GLN:HG3	1:A:474:MET:SD	2.51	0.51
1:A:312:ILE:HG22	1:A:313:VAL:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ILE:HG12	1:B:307:LEU:HD13	1.92	0.50
1:B:335:ASP:C	1:B:337:ALA:H	2.13	0.50
1:B:336:LEU:C	1:B:495:PHE:HZ	2.15	0.50
1:B:412:ALA:O	1:B:413:GLN:C	2.49	0.50
1:B:473:LYS:HE2	1:B:488:ASP:CG	2.30	0.50
1:A:251:PHE:CD1	1:A:251:PHE:C	2.85	0.50
1:A:323:SER:HB2	1:B:323:SER:OG	2.12	0.50
1:A:458:ASN:CG	1:A:459:GLY:H	2.13	0.50
1:A:467:VAL:HG12	1:A:468:CYS:N	2.27	0.50
1:A:473:LYS:HB2	1:A:484:PHE:CD2	2.46	0.50
1:B:306:TYR:CE2	1:B:310:CYS:SG	3.05	0.50
1:A:187:LEU:O	1:A:202:SER:HB2	2.12	0.50
1:A:267:LEU:O	1:A:283:GLN:CA	2.60	0.49
1:A:407:ILE:N	1:A:409:TYR:HE2	2.09	0.49
1:B:250:ARG:HG2	1:B:250:ARG:NH1	2.07	0.49
1:B:148:GLN:CA	1:B:151:ARG:HB3	2.42	0.49
1:B:269:MET:CE	1:B:300:GLU:O	2.56	0.49
1:A:148:GLN:O	1:A:151:ARG:N	2.46	0.49
1:B:196:ASN:HD22	1:B:196:ASN:N	2.10	0.49
1:B:199:PHE:C	1:B:200:LEU:HD23	2.32	0.49
1:A:173:PHE:O	1:A:176:ILE:HG12	2.11	0.49
1:A:519:ARG:HB2	1:A:519:ARG:CZ	2.42	0.49
1:B:163:LEU:HD22	1:B:317:ALA:HA	1.94	0.49
1:A:107:ASP:OD1	1:A:194:SER:HB3	2.13	0.49
1:A:426:ASP:HB2	1:A:449:ARG:HG3	1.94	0.49
1:B:172:ILE:HD13	1:B:310:CYS:SG	2.53	0.49
1:A:107:ASP:O	1:A:193:ASP:HA	2.13	0.49
1:A:425:PRO:HA	1:A:483:PRO:HB3	1.93	0.49
1:B:193:ASP:O	1:B:194:SER:C	2.51	0.49
1:B:370:PHE:CE2	1:B:412:ALA:HB2	2.48	0.49
1:A:172:ILE:HD13	1:A:310:CYS:SG	2.53	0.49
1:A:498:PHE:O	1:A:499:CYS:C	2.49	0.49
1:B:221:ILE:HG22	1:B:222:ARG:N	2.27	0.49
1:A:189:LEU:HD12	1:A:190:VAL:N	2.26	0.48
1:A:309:PHE:CE2	1:B:157:LYS:HD3	2.48	0.48
1:A:454:THR:CG2	1:A:455:PRO:CD	2.91	0.48
1:B:411:TYR:CE2	1:B:432:ARG:HD3	2.48	0.48
1:B:472:ASN:HB3	1:B:481:VAL:CG2	2.43	0.48
1:A:418:THR:CG2	1:A:420:GLU:H	2.27	0.48
1:A:427:VAL:C	1:A:429:LYS:H	2.16	0.48
1:B:427:VAL:HG21	1:B:448:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:N	1:A:409:TYR:CE2	2.82	0.48
1:A:422:LEU:CD2	1:A:424:ILE:CD1	2.86	0.48
1:A:203:ARG:HB3	1:A:216:VAL:HG13	1.96	0.48
1:B:340:ILE:HG22	1:B:341:PHE:N	2.27	0.48
1:A:251:PHE:CE1	1:A:252:ASN:O	2.66	0.48
1:A:296:THR:N	1:A:299:ASP:HB2	2.29	0.48
1:A:414:TYR:CD2	1:A:414:TYR:C	2.87	0.48
1:B:250:ARG:NH1	1:B:250:ARG:HG3	2.26	0.48
1:B:466:GLY:O	1:B:467:VAL:HG23	2.14	0.48
1:A:267:LEU:HB2	1:A:295:PHE:CD2	2.48	0.47
1:B:428:SER:C	1:B:429:LYS:HG3	2.34	0.47
1:B:497:ILE:HG22	1:B:498:PHE:N	2.28	0.47
1:B:450:SER:OG	1:B:472:ASN:N	2.47	0.47
1:B:458:ASN:CB	1:B:465:ILE:HG13	2.43	0.47
1:B:473:LYS:HB3	1:B:482:LYS:O	2.15	0.47
1:A:233:VAL:O	1:A:234:ALA:C	2.53	0.47
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.96	0.47
1:B:207:VAL:O	1:B:208:ALA:O	2.33	0.47
1:B:373:ASP:OD1	1:B:376:CYS:N	2.46	0.47
1:A:200:LEU:H	1:A:200:LEU:HD23	1.79	0.47
1:B:427:VAL:HG11	1:B:448:ILE:O	2.14	0.47
1:A:174:LEU:HD12	1:A:174:LEU:O	2.15	0.47
1:A:198:LYS:O	1:A:199:PHE:CB	2.63	0.47
1:A:205:PHE:CZ	1:A:215:GLU:O	2.68	0.47
1:A:414:TYR:HE2	1:A:418:THR:HG1	1.61	0.47
1:B:272:LYS:HG3	1:B:278:VAL:HA	1.95	0.47
1:A:275:ARG:O	1:A:276:GLU:HB2	2.15	0.47
1:A:179:LEU:HD11	1:A:303:PHE:HA	1.96	0.47
1:A:189:LEU:HD12	1:A:189:LEU:C	2.34	0.47
1:B:191:CYS:HB2	1:B:199:PHE:CE1	2.50	0.46
1:A:153:LEU:HD23	1:B:153:LEU:HD23	1.95	0.46
1:A:238:GLU:HB3	1:A:239:PRO:HD2	1.97	0.46
1:A:243:LYS:HE3	1:A:243:LYS:HB2	1.61	0.46
1:A:458:ASN:CG	1:A:459:GLY:N	2.67	0.46
1:B:164:ASP:OD1	1:B:166:THR:HB	2.16	0.46
1:A:275:ARG:NH1	1:A:275:ARG:CG	2.79	0.46
1:A:432:ARG:HB3	1:A:433:PHE:CD1	2.50	0.46
1:A:500:GLY:O	1:A:501:LEU:C	2.53	0.46
1:A:373:ASP:HA	1:A:381:SER:OG	2.14	0.46
1:B:296:THR:O	1:B:298:LYS:N	2.49	0.46
1:B:452:LEU:HD12	1:B:452:LEU:C	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:O	1:B:505:ASN:N	2.49	0.46
1:A:486:ARG:O	1:A:490:GLN:HB2	2.16	0.46
1:B:389:GLU:O	1:B:390:GLU:HB2	2.16	0.46
1:A:334:LEU:O	1:A:337:ALA:HB3	2.15	0.46
1:B:107:ASP:OD1	1:B:194:SER:OG	2.32	0.46
1:B:151:ARG:NH1	1:B:154:GLU:OE1	2.49	0.46
1:B:246:TYR:CE2	1:B:262:LYS:HD2	2.51	0.46
1:A:336:LEU:N	1:A:336:LEU:HD23	2.31	0.46
1:A:461:LYS:HE3	1:A:461:LYS:O	2.16	0.46
1:B:148:GLN:O	1:B:152:LEU:N	2.39	0.46
1:B:342:GLU:CG	1:B:343:GLU:HG3	2.42	0.46
1:B:380:PHE:O	1:B:381:SER:C	2.55	0.46
1:A:225:TRP:O	1:A:226:ASN:CB	2.64	0.46
1:A:418:THR:O	1:A:419:MET:HB2	2.15	0.46
1:B:196:ASN:N	1:B:196:ASN:ND2	2.64	0.46
1:A:344:GLN:H	1:B:505:ASN:HD21	1.65	0.45
1:B:320:TYR:O	1:B:323:SER:HB3	2.16	0.45
1:B:514:ARG:O	1:B:514:ARG:HG2	2.14	0.45
1:A:426:ASP:OD1	1:A:427:VAL:N	2.48	0.45
1:B:368:THR:CB	1:B:370:PHE:HE1	2.30	0.45
1:B:474:MET:CE	1:B:479:GLY:HA2	2.46	0.45
1:A:303:PHE:O	1:A:307:LEU:HG	2.16	0.45
1:A:231:GLY:O	1:A:234:ALA:HB3	2.17	0.45
1:B:381:SER:O	1:B:382:SER:HB3	2.16	0.45
1:B:494:ALA:HA	1:B:497:ILE:HD12	1.98	0.45
1:B:230:VAL:CG2	1:B:231:GLY:H	2.29	0.45
1:A:287:LYS:HG3	1:A:288:LYS:O	2.17	0.45
1:B:503:ILE:O	1:B:504:GLN:C	2.55	0.45
1:A:373:ASP:OD1	1:A:373:ASP:C	2.55	0.45
1:A:452:LEU:CB	1:A:484:PHE:CE1	3.00	0.45
1:B:373:ASP:HB3	1:B:379:SER:HB2	1.95	0.45
1:B:431:LYS:O	1:B:432:ARG:HG3	2.17	0.45
1:B:458:ASN:CB	1:B:465:ILE:CD1	2.92	0.45
1:B:458:ASN:HD22	1:B:463:LYS:H	1.63	0.45
1:A:414:TYR:C	1:A:414:TYR:HD2	2.20	0.45
1:B:195:SER:O	1:B:196:ASN:CB	2.65	0.45
1:A:153:LEU:O	1:A:154:GLU:C	2.55	0.45
1:B:419:MET:O	1:B:420:GLU:HG2	2.17	0.45
1:B:271:ILE:HG13	1:B:307:LEU:HD13	1.99	0.44
1:A:262:LYS:HD2	1:A:262:LYS:C	2.37	0.44
1:A:314:LEU:O	1:A:317:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ARG:NH1	1:B:277:GLU:OE2	2.49	0.44
1:B:306:TYR:CG	1:B:306:TYR:O	2.69	0.44
1:A:205:PHE:CE1	1:A:215:GLU:O	2.71	0.44
1:A:327:ASN:HD22	1:B:330:ASN:ND2	2.16	0.44
1:A:358:ILE:O	1:A:360:SER:N	2.51	0.44
1:B:456:ILE:O	1:B:456:ILE:HG22	2.17	0.44
1:B:188:PHE:CE2	1:B:202:SER:HB3	2.53	0.44
1:B:233:VAL:O	1:B:237:GLY:N	2.50	0.44
1:B:350:ILE:CG2	1:B:351:LEU:N	2.79	0.44
1:A:251:PHE:CE2	1:A:263:THR:HG21	2.43	0.44
1:A:346:SER:O	1:A:347:LEU:C	2.56	0.44
1:A:272:LYS:HB3	1:A:277:GLU:O	2.18	0.44
1:A:287:LYS:HB2	1:A:295:PHE:CE1	2.53	0.44
1:A:358:ILE:C	1:A:360:SER:N	2.70	0.44
1:B:411:TYR:HE2	1:B:432:ARG:HD3	1.81	0.44
1:A:114:VAL:HG23	1:A:123:SER:O	2.18	0.43
1:A:200:LEU:CD2	1:A:200:LEU:H	2.29	0.43
1:A:358:ILE:HD11	1:A:495:PHE:HE2	1.83	0.43
1:A:105:GLU:OE1	1:B:130:LYS:HB3	2.18	0.43
1:A:242:ILE:H	1:A:242:ILE:HG12	1.49	0.43
1:A:251:PHE:CE1	1:A:253:ALA:CA	2.97	0.43
1:A:281:VAL:HG12	1:A:282:ALA:N	2.34	0.43
1:B:253:ALA:O	1:B:254:GLU:C	2.56	0.43
1:A:269:MET:HE3	1:A:303:PHE:CD1	2.53	0.43
1:A:467:VAL:CG1	1:A:468:CYS:N	2.82	0.43
1:B:244:ASP:HA	1:B:264:GLN:O	2.19	0.43
1:B:336:LEU:O	1:B:495:PHE:CE2	2.68	0.43
1:B:168:LEU:HD22	1:B:313:VAL:HG12	2.00	0.43
1:B:486:ARG:NH1	1:B:486:ARG:CG	2.80	0.43
1:B:320:TYR:CE2	1:B:324:LEU:HD11	2.54	0.43
1:B:370:PHE:CE2	1:B:412:ALA:CB	3.02	0.43
1:A:327:ASN:ND2	1:B:330:ASN:ND2	2.66	0.43
1:B:389:GLU:O	1:B:390:GLU:CB	2.67	0.43
1:A:328:LYS:CE	1:B:129:GLU:HB3	2.49	0.43
1:A:456:ILE:CG2	1:A:500:GLY:HA2	2.48	0.43
1:A:251:PHE:HE1	1:A:253:ALA:CA	2.18	0.43
1:A:478:THR:CG2	1:A:480:LYS:N	2.39	0.43
1:B:155:LEU:CD2	1:B:175:HIS:CG	3.00	0.43
1:B:218:ASN:HB3	1:B:219:ASN:H	1.70	0.43
1:A:251:PHE:CD1	1:A:252:ASN:N	2.87	0.42
1:B:188:PHE:CD2	1:B:202:SER:CB	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:HG22	1:A:479:GLY:N	2.33	0.42
1:B:390:GLU:HB3	1:B:391:LEU:H	1.56	0.42
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.60	0.42
1:A:344:GLN:O	1:A:506:THR:HA	2.19	0.42
1:A:470:LEU:CD2	1:A:492:LEU:CD1	2.96	0.42
1:A:475:GLU:OE1	1:A:482:LYS:HD3	2.19	0.42
1:A:147:ASP:HA	1:A:150:SER:HB3	2.00	0.42
1:A:168:LEU:HD21	1:A:314:LEU:HA	2.02	0.42
1:A:344:GLN:NE2	1:A:505:ASN:HB2	2.35	0.42
1:B:174:LEU:O	1:B:175:HIS:C	2.54	0.42
1:A:287:LYS:CD	1:A:294:THR:O	2.65	0.42
1:A:334:LEU:HD21	1:B:334:LEU:HG	2.00	0.42
1:A:433:PHE:O	1:A:434:PRO:C	2.56	0.42
1:B:153:LEU:C	1:B:155:LEU:N	2.71	0.42
1:B:354:ILE:O	1:B:358:ILE:CG1	2.66	0.42
1:B:510:GLU:HA	1:B:513:GLU:HB2	2.02	0.42
1:A:378:ASP:OD2	1:A:379:SER:CB	2.63	0.42
1:B:370:PHE:HD2	1:B:380:PHE:CE1	2.38	0.42
1:A:153:LEU:HD21	1:B:153:LEU:CG	2.39	0.42
1:A:422:LEU:HD23	1:A:424:ILE:CG1	2.50	0.42
1:B:427:VAL:HG21	1:B:448:ILE:CG2	2.50	0.42
1:A:449:ARG:NH1	1:A:449:ARG:HB2	2.35	0.42
1:A:481:VAL:O	1:A:481:VAL:HG12	2.20	0.42
1:B:122:VAL:O	1:B:122:VAL:HG23	2.20	0.42
1:A:366:LYS:HD3	1:A:385:HIS:HE1	1.80	0.42
1:B:113:ILE:HG21	1:B:490:GLN:O	2.20	0.42
1:B:173:PHE:CE2	1:B:204:LEU:HB3	2.55	0.42
1:B:476:GLU:O	1:B:477:ASN:CB	2.59	0.42
1:B:491:PHE:CE2	1:B:495:PHE:CD1	3.05	0.42
1:A:219:ASN:HD22	1:A:219:ASN:HA	1.67	0.41
1:A:306:TYR:CD2	1:A:306:TYR:O	2.72	0.41
1:A:207:VAL:HG23	1:A:208:ALA:O	2.20	0.41
1:A:409:TYR:HD2	1:A:409:TYR:N	2.08	0.41
1:B:499:CYS:O	1:B:500:GLY:C	2.57	0.41
1:A:248:ASP:HA	1:A:249:PRO:HD2	1.88	0.41
1:A:505:ASN:HD21	1:B:343:GLU:HA	1.86	0.41
1:A:512:VAL:CG2	1:B:509:TYR:HE1	2.30	0.41
1:B:252:ASN:C	1:B:252:ASN:HD22	2.22	0.41
1:A:190:VAL:HG12	1:A:191:CYS:N	2.35	0.41
1:A:418:THR:O	1:A:420:GLU:HG3	2.20	0.41
1:B:230:VAL:O	1:B:233:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:MET:HE3	1:B:479:GLY:HA2	2.01	0.41
1:A:168:LEU:CD2	1:A:314:LEU:HA	2.50	0.41
1:A:365:GLN:HB2	1:A:472:ASN:HB2	2.03	0.41
1:A:117:ASP:O	1:A:120:GLY:HA2	2.20	0.41
1:A:291:ASN:N	1:A:291:ASN:ND2	2.68	0.41
1:A:384:PHE:C	1:A:384:PHE:CD2	2.94	0.41
1:B:193:ASP:C	1:B:195:SER:N	2.72	0.41
1:B:380:PHE:HE1	1:B:412:ALA:HB1	1.86	0.41
1:B:474:MET:HE2	1:B:474:MET:HB2	1.84	0.41
1:B:111:ARG:HE	1:B:111:ARG:HB3	1.47	0.41
1:B:148:GLN:CB	1:B:151:ARG:HB3	2.49	0.41
1:B:359:ILE:HG23	1:B:364:VAL:HG23	2.03	0.41
1:A:190:VAL:HG23	1:A:279:VAL:C	2.41	0.41
1:A:302:ASP:OD2	1:A:302:ASP:N	2.54	0.41
1:A:345:GLN:HE22	1:B:505:ASN:ND2	2.19	0.41
1:A:357:THR:HG22	1:A:358:ILE:N	2.36	0.41
1:B:207:VAL:O	1:B:208:ALA:C	2.59	0.41
1:B:236:LEU:HD22	1:B:236:LEU:HA	1.91	0.41
1:B:275:ARG:HH11	1:B:277:GLU:CD	2.16	0.41
1:B:365:GLN:HG3	1:B:474:MET:SD	2.61	0.41
1:B:375:ASP:O	1:B:376:CYS:HB2	2.21	0.41
1:B:393:LYS:O	1:B:394:SER:CB	2.61	0.41
1:A:362:MET:SD	1:A:492:LEU:CD1	3.09	0.41
1:B:155:LEU:HD22	1:B:175:HIS:ND1	2.36	0.40
1:B:194:SER:HB3	1:B:487:ASN:H	1.85	0.40
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.87	0.40
1:A:458:ASN:H	1:A:458:ASN:HD22	1.69	0.40
1:A:269:MET:CE	1:A:303:PHE:CD1	3.04	0.40
1:A:459:GLY:HA3	1:B:342:GLU:OE2	2.22	0.40
1:B:108:ARG:CB	1:B:109:PRO:CD	2.96	0.40
1:B:358:ILE:HG12	1:B:358:ILE:H	1.59	0.40
1:B:458:ASN:HB3	1:B:465:ILE:HG12	1.99	0.40
1:B:227:LYS:O	1:B:231:GLY:HA3	2.21	0.40
1:B:331:GLN:O	1:B:335:ASP:HB2	2.22	0.40
1:B:418:THR:O	1:B:419:MET:CB	2.68	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	370/432 (86%)	279 (75%)	65 (18%)	26 (7%)	1 7
1	B	359/432 (83%)	268 (75%)	57 (16%)	34 (10%)	0 3
All	All	729/864 (84%)	547 (75%)	122 (17%)	60 (8%)	1 5

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
1	A	208	ALA
1	A	216	VAL
1	A	480	LYS
1	B	103	ALA
1	B	118	SER
1	B	119	GLU
1	B	127	ASP
1	B	305	ALA
1	B	390	GLU
1	B	448	ILE
1	B	465	ILE
1	B	504	GLN
1	A	120	GLY
1	A	149	SER
1	A	213	LEU
1	A	231	GLY
1	A	234	ALA
1	A	289	SER
1	A	409	TYR
1	A	478	THR
1	A	512	VAL
1	B	273	ASN
1	B	292	GLY
1	B	302	ASP

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Mol	Chain	Res	Type
1	B	340	ILE
1	B	377	SER
1	B	381	SER
1	B	459	GLY
1	B	478	THR
1	B	500	GLY
1	B	519	ARG
1	A	119	GLU
1	A	408	ASN
1	A	428	SER
1	A	460	LYS
1	A	511	ALA
1	B	149	SER
1	B	419	MET
1	B	433	PHE
1	B	457	LYS
1	B	477	ASN
1	A	347	LEU
1	A	455	PRO
1	B	294	THR
1	B	346	SER
1	B	412	ALA
1	A	177	HIS
1	A	472	ASN
1	A	487	ASN
1	B	297	GLU
1	B	425	PRO
1	B	482	LYS
1	A	199	PHE
1	A	233	VAL
1	B	231	GLY
1	B	503	ILE
1	B	221	ILE
1	A	372	VAL
1	B	229	ILE

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	338/388 (87%)	247 (73%)	91 (27%)	0 1
1	B	331/388 (85%)	240 (72%)	91 (28%)	0 1
All	All	669/776 (86%)	487 (73%)	182 (27%)	0 1

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	SER
1	A	105	GLU
1	A	108	ARG
1	A	122	VAL
1	A	123	SER
1	A	126	SER
1	A	127	ASP
1	A	149	SER
1	A	150	SER
1	A	151	ARG
1	A	152	LEU
1	A	160	SER
1	A	163	LEU
1	A	174	LEU
1	A	179	LEU
1	A	181	SER
1	A	189	LEU
1	A	195	SER
1	A	200	LEU
1	A	205	PHE
1	A	212	THR
1	A	215	GLU
1	A	219	ASN
1	A	227	LYS
1	A	230	VAL
1	A	236	LEU
1	A	241	ASN
1	A	242	ILE
1	A	243	LYS
1	A	248	ASP
1	A	252	ASN
1	A	259	THR
1	A	262	LYS
1	A	269	MET

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Mol	Chain	Res	Type
1	A	272	LYS
1	A	275	ARG
1	A	283	GLN
1	A	291	ASN
1	A	294	THR
1	A	296	THR
1	A	298	LYS
1	A	299	ASP
1	A	314	LEU
1	A	323	SER
1	A	327	ASN
1	A	328	LYS
1	A	333	LEU
1	A	336	LEU
1	A	338	SER
1	A	339	LEU
1	A	347	LEU
1	A	349	VAL
1	A	357	THR
1	A	360	SER
1	A	371	ILE
1	A	376	CYS
1	A	377	SER
1	A	379	SER
1	A	381	SER
1	A	382	SER
1	A	386	MET
1	A	389	GLU
1	A	392	GLU
1	A	407	ILE
1	A	408	ASN
1	A	409	TYR
1	A	410	MET
1	A	414	TYR
1	A	418	THR
1	A	420	GLU
1	A	422	LEU
1	A	426	ASP
1	A	427	VAL
1	A	431	LYS
1	A	446	GLN
1	A	448	ILE

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Mol	Chain	Res	Type
1	A	449	ARG
1	A	452	LEU
1	A	453	CYS
1	A	457	LYS
1	A	458	ASN
1	A	461	LYS
1	A	462	ASN
1	A	463	LYS
1	A	470	LEU
1	A	482	LYS
1	A	485	ASN
1	A	487	ASN
1	A	492	LEU
1	A	513	GLU
1	A	516	MET
1	B	101	ILE
1	B	104	SER
1	B	108	ARG
1	B	111	ARG
1	B	116	LYS
1	B	117	ASP
1	B	119	GLU
1	B	128	SER
1	B	130	LYS
1	B	148	GLN
1	B	149	SER
1	B	151	ARG
1	B	161	SER
1	B	171	LYS
1	B	172	ILE
1	B	180	ILE
1	B	187	LEU
1	B	194	SER
1	B	196	ASN
1	B	199	PHE
1	B	200	LEU
1	B	219	ASN
1	B	223	LEU
1	B	227	LYS
1	B	233	VAL
1	B	236	LEU
1	B	243	LYS

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Mol	Chain	Res	Type
1	B	248	ASP
1	B	250	ARG
1	B	252	ASN
1	B	254	GLU
1	B	262	LYS
1	B	272	LYS
1	B	276	GLU
1	B	277	GLU
1	B	291	ASN
1	B	294	THR
1	B	301	LYS
1	B	303	PHE
1	B	307	LEU
1	B	318	GLN
1	B	331	GLN
1	B	335	ASP
1	B	338	SER
1	B	339	LEU
1	B	342	GLU
1	B	343	GLU
1	B	346	SER
1	B	347	LEU
1	B	348	GLU
1	B	357	THR
1	B	358	ILE
1	B	370	PHE
1	B	372	VAL
1	B	374	GLU
1	B	378	ASP
1	B	384	PHE
1	B	387	GLU
1	B	389	GLU
1	B	390	GLU
1	B	391	LEU
1	B	393	LYS
1	B	394	SER
1	B	409	TYR
1	B	410	MET
1	B	416	LYS
1	B	418	THR
1	B	424	ILE
1	B	427	VAL

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Mol	Chain	Res	Type
1	B	430	ASP
1	B	431	LYS
1	B	432	ARG
1	B	433	PHE
1	B	447	CYS
1	B	449	ARG
1	B	452	LEU
1	B	453	CYS
1	B	460	LYS
1	B	462	ASN
1	B	463	LYS
1	B	465	ILE
1	B	470	LEU
1	B	474	MET
1	B	475	GLU
1	B	476	GLU
1	B	480	LYS
1	B	495	PHE
1	B	501	LEU
1	B	512	VAL
1	B	516	MET
1	B	519	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	177	HIS
1	A	219	ASN
1	A	241	ASN
1	A	252	ASN
1	A	274	HIS
1	A	291	ASN
1	A	315	HIS
1	A	363	GLN
1	A	408	ASN
1	A	462	ASN
1	A	485	ASN
1	A	505	ASN
1	B	177	HIS
1	B	196	ASN
1	B	219	ASN

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Mol	Chain	Res	Type
1	B	252	ASN
1	B	257	GLN
1	B	291	ASN
1	B	327	ASN
1	B	330	ASN
1	B	345	GLN
1	B	363	GLN
1	B	385	HIS
1	B	458	ASN
1	B	462	ASN
1	B	477	ASN
1	B	505	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	378/432 (87%)	-0.39	7 (1%)	66	46	57, 95, 142, 178	0
1	B	369/432 (85%)	-0.33	8 (2%)	62	41	58, 97, 140, 179	0
All	All	747/864 (86%)	-0.36	15 (2%)	65	44	57, 96, 142, 179	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	GLU	9.3
1	B	130	LYS	6.9
1	A	212	THR	6.7
1	A	211	SER	6.0
1	B	128	SER	4.6
1	A	392	GLU	4.6
1	A	213	LEU	4.5
1	A	209	GLU	3.8
1	B	477	ASN	3.3
1	A	210	GLY	3.2
1	A	391	LEU	2.9
1	B	391	LEU	2.8
1	B	394	SER	2.6
1	B	520	ASN	2.2
1	B	390	GLU	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.