Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 06:45 PM EST

PDB ID	:	3FIP
Title	:	Crystal structure of Usher PapC translocation pore
Authors	:	Huang, Y.; Deisenhofer, J.
Deposited on	:	2008-12-12
Resolution	:	3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

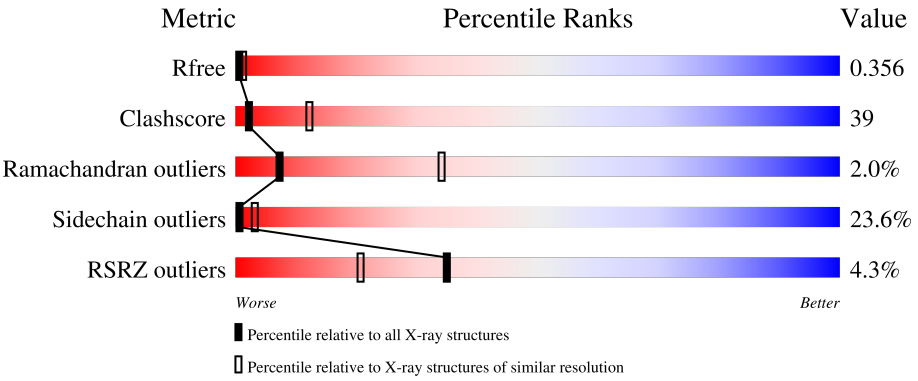
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	493	2% 37% 40% 12% 12%
1	B	493	5% 29% 37% 11% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6295 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 Outer membrane usher protein papC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	14	0	0
			3387	2115	605	661	6			
1	B	384	Total	C	N	O	S	4	0	0
			2908	1817	516	569	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	SER	-	expression tag	UNP P07110
A	625	PHE	-	expression tag	UNP P07110
A	626	GLY	-	expression tag	UNP P07110
A	627	VAL	-	expression tag	UNP P07110
A	628	SER	-	expression tag	UNP P07110
A	629	ALA	-	expression tag	UNP P07110
A	630	SER	-	expression tag	UNP P07110
A	631	GLY	-	expression tag	UNP P07110
A	632	GLY	-	expression tag	UNP P07110
A	633	ALA	-	expression tag	UNP P07110
A	634	THR	-	expression tag	UNP P07110
A	635	ILE	-	expression tag	UNP P07110
A	636	THR	-	expression tag	UNP P07110
B	624	SER	-	expression tag	UNP P07110
B	625	PHE	-	expression tag	UNP P07110
B	626	GLY	-	expression tag	UNP P07110
B	627	VAL	-	expression tag	UNP P07110
B	628	SER	-	expression tag	UNP P07110
B	629	ALA	-	expression tag	UNP P07110
B	630	SER	-	expression tag	UNP P07110
B	631	GLY	-	expression tag	UNP P07110
B	632	GLY	-	expression tag	UNP P07110
B	633	ALA	-	expression tag	UNP P07110
B	634	THR	-	expression tag	UNP P07110
B	635	ILE	-	expression tag	UNP P07110

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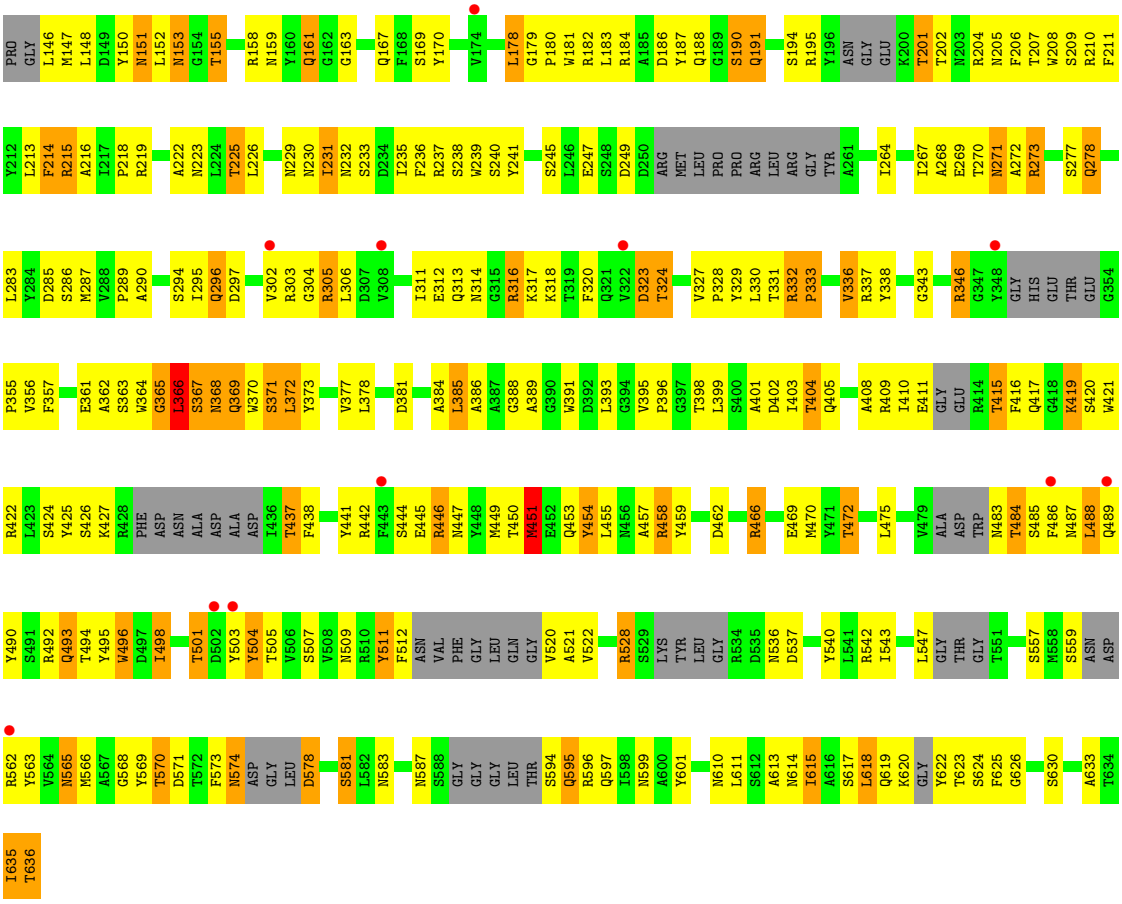
Chain	Residue	Modelled	Actual	Comment	Reference
B	636	THR	-	expression tag	UNP P07110

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.

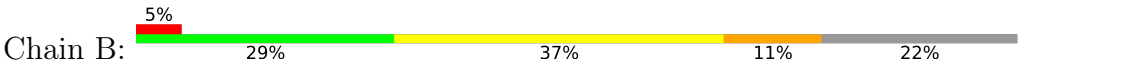
• Molecule 1: Outer membrane usher protein papC

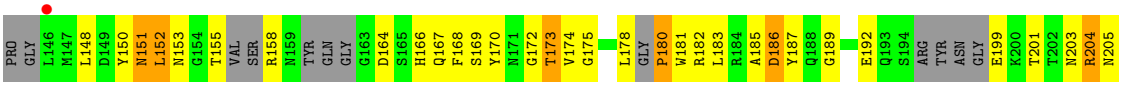
Chain A:

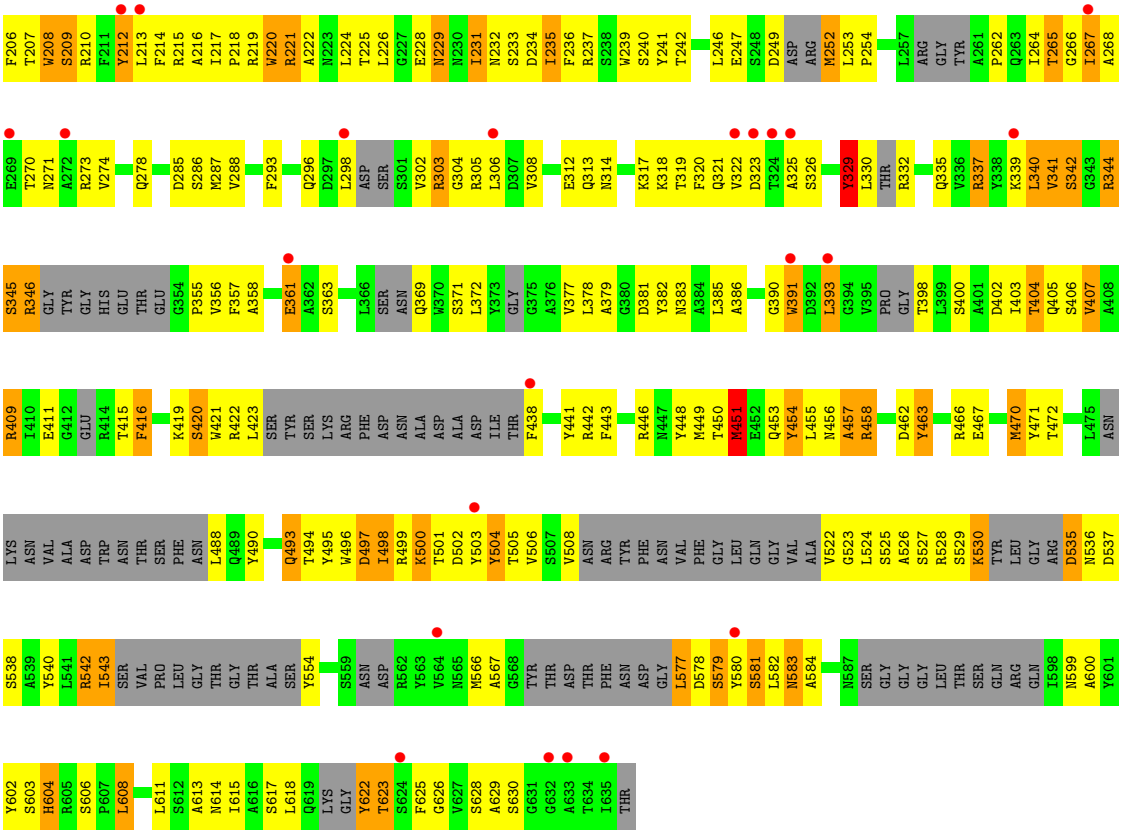


• Molecule 1: Outer membrane usher protein papC

Chain B:






F206 T207 W208 S209 R210 F211 Y212 L213 F214 R215 A216 I217 P218 R219 W220 R221 A222 N223 L224 T225 L226 G227 E228 N229 N230 I231 N232 S233 D234 I235 F236 R237 S238 W239 S240 Y241 T242 L246 E247 S248 D249 ASP ARG M252 L253 P254 L257 ARG GLY TYR A261 P262 Q263 I264 T265 G266 I267 A268
E269 T270 N271 A272 R273 V274 Q278 D285 S286 M287 V288 F293 Q296 D297 L298 ASP SER S301 V302 R303 G304 R305 L306 D307 V308 E312 Q313 N314 K317 K318 T319 F320 Q321 V322 D323 T324 A325 S326 Y329 L330 THR R332 Q335 V336 R337 Y338 K339 L340 V341 S342 G343 R344
S345 R346 GLY TYR GLY HIS GLU THR GLU G354 P355 V356 F357 A358 E361 A362 S363 L366 SER ASN Q369 W370 S371 L372 Y373 GLY G375 A376 V377 L378 A379 G380 D381 Y382 N383 A384 L385 A386 G390 W391 D392 L393 G394 V395 PRO GLY T398 L399 S400 A401 D402 I403 T404 Q405 S406 V407 A408
R409 I410 E411 G412 GLU R414 T415 F416 K419 S420 W421 R422 L423 SER TYR SER LYS ARG PHE ASP ASN ALA ASP ALA ASP ILE THR F438 Y441 R442 F443 R446 N447 Y448 M449 T450 N451 E452 Q453 Y454 L455 N456 A457 R458 D462 Y463 R466 E467 M470 Y471 T472 L475 ASN
LYS ASN VAL ALA ASP TRP ASN THR SER PHE ASN L488 Q489 Y490 Q493 T494 Y495 W496 D497 I498 R499 K500 T501 D502 Y503 Y504 T505 V506 S507 V508 ASN ARG TYR PHE ASN VAL PHE GLY LEU GLN GLY VAL ALA V522 G523 L524 S525 A526 S527 R528 S529 K530 TYR LEU GLY ARG D535 N536 D537
S538 A539 Y540 L541 R542 I543 SER VAL PRO LEU GLY THR GLY THR ALA SER Y554 S559 ASN ASP R562 Y563 V564 N565 M566 A567 G568 TYR THR ASP THR PHE ASN ASP GLY L577 D578 S579 Y580 S581 L582 N583 A584 W587 SER GLY GLY GLY LEU THR SER GLN ARG GLN I598 N599 A600 Y601
Y602 S603 H604 R605 S606 P607 L608 L611 S612 A613 N614 I615 A616 S617 L618 Q619 LYS GLY Y622 T623 S624 F625 G626 V627 S628 A629 S630 G631 G632 A633 T634 I635 THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.04Å 120.04Å 354.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.15 49.68 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.68-3.15) 98.0 (49.68-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.285 , 0.359 0.289 , 0.356	Depositor DCC
R_{free} test set	1151 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	115.3	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 106.5	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	0.88	EDS
Total number of atoms	6295	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.59	1/3450 (0.0%)	0.83	14/4668 (0.3%)
1	B	0.44	0/2946	0.83	13/3971 (0.3%)
All	All	0.52	1/6396 (0.0%)	0.83	27/8639 (0.3%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	SER	CB-OG	15.64	1.62	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	LYS	N-CA-C	-14.12	72.88	111.00
1	B	317	LYS	CB-CA-C	13.85	138.10	110.40
1	A	190	SER	CB-CA-C	-11.41	88.42	110.10
1	B	579	SER	CB-CA-C	-11.02	89.16	110.10
1	B	318	LYS	N-CA-C	-10.61	82.35	111.00
1	B	580	TYR	N-CA-CB	-10.07	92.47	110.60
1	A	485	SER	N-CA-CB	9.69	125.04	110.50
1	A	317	LYS	N-CA-C	-9.56	85.19	111.00
1	A	366	LEU	CB-CA-C	-9.43	92.29	110.20
1	A	317	LYS	CB-CA-C	9.30	129.01	110.40
1	A	191	GLN	N-CA-CB	-8.92	94.54	110.60
1	B	318	LYS	N-CA-CB	7.39	123.91	110.60
1	A	316	ARG	CB-CA-C	7.33	125.06	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	TRP	CB-CA-C	7.15	124.71	110.40
1	B	209	SER	N-CA-C	-7.11	91.80	111.00
1	A	296	GLN	CB-CA-C	-6.90	96.60	110.40
1	B	208	TRP	N-CA-C	-6.81	92.62	111.00
1	A	318	LYS	N-CA-C	-6.67	92.98	111.00
1	A	484	THR	CB-CA-C	6.40	128.87	111.60
1	B	180	PRO	N-CA-CB	6.07	110.58	103.30
1	A	316	ARG	N-CA-C	-5.96	94.92	111.00
1	B	287	MET	CB-CA-C	5.75	121.90	110.40
1	A	365	GLY	N-CA-C	-5.56	99.19	113.10
1	A	296	GLN	N-CA-C	5.36	125.47	111.00
1	A	366	LEU	N-CA-C	-5.31	96.67	111.00
1	B	209	SER	N-CA-CB	5.06	118.10	110.50
1	B	385	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	SER	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	3387	0	3176	239	0
1	B	2908	0	2695	238	0
All	All	6295	0	5871	476	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 39.

All (476) 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:267:ILE:HG22	1:B:268:ALA:H	1.10	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:HG2	1:A:332:ARG:HH11	1.14	1.07
1:B:614:ASN:HB3	1:B:626:GLY:HA3	1.32	1.04
1:A:570:THR:HB	1:A:581:SER:HB3	1.35	1.03
1:A:161:GLN:H	1:A:161:GLN:HE21	1.08	1.00
1:B:466:ARG:HB3	1:B:496:TRP:HD1	1.26	1.00
1:A:153:ASN:HD22	1:A:153:ASN:N	1.56	0.99
1:B:554:TYR:HA	1:B:567:ALA:HA	1.47	0.97
1:A:147:MET:HG2	1:A:148:LEU:H	1.27	0.97
1:B:391:TRP:HE1	1:B:393:LEU:HG	1.28	0.95
1:A:449:MET:HG3	1:A:466:ARG:HH22	1.35	0.92
1:A:403:ILE:HD12	1:A:421:TRP:CD1	2.07	0.89
1:B:240:SER:HB2	1:B:346:ARG:NH1	1.88	0.88
1:B:267:ILE:HG22	1:B:268:ALA:N	1.88	0.88
1:B:151:ASN:HD22	1:B:152:LEU:N	1.71	0.88
1:B:490:TYR:CD1	1:B:504:TYR:HB2	2.10	0.87
1:A:240:SER:HB3	1:A:346:ARG:HH12	1.39	0.87
1:A:332:ARG:HH11	1:A:332:ARG:CG	1.87	0.86
1:A:368:ASN:HD22	1:A:369:GLN:NE2	1.72	0.86
1:A:346:ARG:HH11	1:A:346:ARG:HB3	1.42	0.84
1:A:446:ARG:HA	1:A:496:TRP:NE1	1.92	0.84
1:B:382:TYR:CE2	1:B:451:MET:HG2	2.14	0.83
1:B:342:SER:HA	1:B:358:ALA:HA	1.61	0.82
1:B:305:ARG:HD3	1:B:321:GLN:CD	2.00	0.82
1:B:490:TYR:HD1	1:B:504:TYR:HB2	1.44	0.81
1:B:267:ILE:CG2	1:B:268:ALA:H	1.91	0.81
1:B:457:ALA:HB1	1:B:463:TYR:CD2	2.16	0.81
1:A:271:ASN:ND2	1:A:599:ASN:HD21	1.79	0.81
1:A:304:GLY:O	1:A:324:THR:HG23	1.81	0.80
1:A:240:SER:HB3	1:A:346:ARG:NH1	1.96	0.80
1:A:194:SER:O	1:A:195:ARG:HG2	1.81	0.80
1:A:368:ASN:HD22	1:A:369:GLN:HE21	1.29	0.80
1:B:239:TRP:HZ2	1:B:357:PHE:CE1	2.00	0.80
1:B:325:ALA:HA	1:B:438:PHE:CE2	2.17	0.80
1:A:159:ASN:HD21	1:A:161:GLN:HG2	1.46	0.80
1:B:175:GLY:HA2	1:B:183:LEU:HD23	1.63	0.79
1:B:151:ASN:HD22	1:B:152:LEU:H	1.28	0.79
1:B:581:SER:O	1:B:582:LEU:HD23	1.83	0.79
1:A:270:THR:OG1	1:A:313:GLN:HG3	1.82	0.78
1:B:488:LEU:HA	1:B:506:VAL:HG22	1.65	0.77
1:B:466:ARG:HB3	1:B:496:TRP:CD1	2.16	0.77
1:A:333:PRO:HG3	1:A:367:SER:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:H	1:A:161:GLN:NE2	1.84	0.76
1:A:332:ARG:HG2	1:A:332:ARG:NH1	1.90	0.76
1:B:303:ARG:NH1	1:B:326:SER:HB2	2.01	0.76
1:A:493:GLN:H	1:A:501:THR:HG22	1.50	0.76
1:A:161:GLN:HE21	1:A:161:GLN:N	1.83	0.75
1:A:437:THR:HB	1:A:475:LEU:HD21	1.68	0.75
1:B:314:ASN:HB3	1:B:622:TYR:CE2	2.22	0.75
1:A:566:MET:HE1	1:A:597:GLN:HG2	1.69	0.74
1:A:152:LEU:C	1:A:153:ASN:HD22	1.90	0.74
1:A:446:ARG:HA	1:A:496:TRP:HE1	1.51	0.74
1:A:386:ALA:HB2	1:A:404:THR:HB	1.70	0.73
1:A:188:GLN:HE21	1:A:209:SER:HB3	1.53	0.73
1:B:330:LEU:HD21	1:B:390:GLY:HA3	1.69	0.73
1:B:342:SER:HB2	1:B:358:ALA:HB2	1.71	0.73
1:B:240:SER:HB2	1:B:346:ARG:HH12	1.51	0.73
1:B:342:SER:HB2	1:B:358:ALA:CB	2.19	0.73
1:B:231:ILE:HD12	1:B:241:TYR:CD2	2.24	0.72
1:B:382:TYR:CD2	1:B:451:MET:HG2	2.24	0.71
1:A:155:THR:HG23	1:A:167:GLN:HB3	1.73	0.71
1:A:416:PHE:HD2	1:A:447:ASN:OD1	1.74	0.70
1:B:457:ALA:HA	1:B:462:ASP:N	2.06	0.70
1:A:159:ASN:HB3	1:A:163:GLY:H	1.56	0.70
1:B:231:ILE:HD11	1:B:341:VAL:HG11	1.72	0.70
1:B:151:ASN:O	1:B:152:LEU:HD23	1.91	0.70
1:A:147:MET:HG3	1:A:633:ALA:O	1.91	0.70
1:B:186:ASP:HB3	1:B:209:SER:HB2	1.73	0.69
1:B:239:TRP:HZ2	1:B:357:PHE:HE1	1.39	0.69
1:A:403:ILE:HD12	1:A:421:TRP:HD1	1.58	0.69
1:B:329:TYR:CD1	1:B:363:SER:HB2	2.28	0.69
1:B:210:ARG:HD2	1:B:229:ASN:ND2	2.08	0.68
1:B:220:TRP:HA	1:B:220:TRP:CE3	2.28	0.68
1:B:421:TRP:O	1:B:442:ARG:HG3	1.93	0.67
1:A:170:TYR:O	1:A:170:TYR:CD2	2.47	0.67
1:A:495:TYR:HB2	1:A:498:ILE:O	1.94	0.67
1:B:215:ARG:O	1:B:215:ARG:HG3	1.94	0.67
1:A:470:MET:CE	1:A:472:THR:HB	2.25	0.67
1:A:573:PHE:O	1:A:574:ASN:ND2	2.27	0.67
1:A:368:ASN:ND2	1:A:369:GLN:NE2	2.43	0.66
1:A:239:TRP:HZ2	1:A:357:PHE:CE1	2.14	0.66
1:B:174:VAL:HG12	1:B:174:VAL:O	1.95	0.66
1:B:457:ALA:HB1	1:B:463:TYR:CG	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:VAL:HG12	1:B:523:GLY:H	1.61	0.66
1:B:402:ASP:OD1	1:B:422:ARG:HD3	1.96	0.66
1:A:398:THR:HB	1:A:426:SER:HB3	1.78	0.65
1:A:147:MET:CG	1:A:148:LEU:H	2.08	0.65
1:A:153:ASN:N	1:A:153:ASN:ND2	2.30	0.65
1:B:170:TYR:O	1:B:170:TYR:CD1	2.50	0.65
1:A:295:ILE:O	1:A:295:ILE:HG22	1.95	0.64
1:A:270:THR:C	1:A:290:ALA:HB2	2.17	0.64
1:B:233:SER:HB2	1:B:361:GLU:OE2	1.97	0.64
1:A:147:MET:HG2	1:A:148:LEU:N	2.07	0.63
1:A:470:MET:HE2	1:A:472:THR:HB	1.81	0.63
1:B:164:ASP:OD2	1:B:166:HIS:HE1	1.82	0.63
1:B:240:SER:CB	1:B:346:ARG:HH12	2.11	0.63
1:A:330:LEU:HD11	1:A:398:THR:HG21	1.81	0.62
1:A:399:LEU:HD12	1:A:424:SER:O	1.99	0.62
1:B:530:LYS:HG2	1:B:535:ASP:OD1	1.99	0.62
1:A:562:ARG:NH1	1:A:587:ASN:HD21	1.97	0.62
1:B:235:ILE:HA	1:B:422:ARG:HH12	1.64	0.62
1:A:269:GLU:HB3	1:A:312:GLU:CD	2.20	0.62
1:A:356:VAL:HG12	1:A:357:PHE:N	2.15	0.62
1:A:475:LEU:HB2	1:A:488:LEU:HD12	1.80	0.62
1:A:159:ASN:ND2	1:A:161:GLN:HG2	2.12	0.62
1:A:346:ARG:HH11	1:A:346:ARG:CB	2.11	0.62
1:B:416:PHE:N	1:B:416:PHE:CD1	2.68	0.62
1:A:336:VAL:HG21	1:A:364:TRP:CD1	2.36	0.61
1:A:183:LEU:HA	1:A:213:LEU:HD23	1.82	0.61
1:A:408:ALA:HB1	1:A:454:TYR:CD1	2.36	0.61
1:B:409:ARG:CB	1:B:415:THR:HG22	2.30	0.61
1:A:225:THR:HG23	1:A:245:SER:OG	2.00	0.61
1:A:330:LEU:HD11	1:A:398:THR:CG2	2.31	0.61
1:B:450:THR:O	1:B:453:GLN:N	2.34	0.61
1:A:240:SER:O	1:A:241:TYR:HB3	2.01	0.60
1:B:525:SER:OG	1:B:540:TYR:HB3	2.01	0.60
1:B:382:TYR:O	1:B:383:ASN:CG	2.40	0.60
1:B:372:LEU:HD12	1:B:372:LEU:O	2.02	0.60
1:A:419:LYS:HG2	1:A:445:GLU:OE1	2.01	0.60
1:B:583:ASN:N	1:B:583:ASN:ND2	2.49	0.59
1:B:178:LEU:HB2	1:B:181:TRP:HB2	1.84	0.59
1:B:614:ASN:O	1:B:615:ILE:HG13	2.02	0.59
1:B:234:ASP:OD2	1:B:339:LYS:NZ	2.29	0.59
1:A:469:GLU:HB2	1:A:494:THR:OG1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ARG:HB3	1:B:415:THR:HG22	1.84	0.59
1:A:181:TRP:CZ3	1:A:215:ARG:HB3	2.37	0.58
1:A:398:THR:HG22	1:A:399:LEU:N	2.18	0.58
1:A:568:GLY:HA3	1:A:583:ASN:OD1	2.03	0.58
1:A:458:ARG:HG2	1:A:458:ARG:O	2.01	0.58
1:A:273:ARG:HH21	1:A:311:ILE:HD13	1.68	0.58
1:A:146:LEU:HB3	1:A:635:ILE:O	2.02	0.58
1:B:153:ASN:ND2	1:B:285:ASP:O	2.36	0.58
1:B:493:GLN:CA	1:B:493:GLN:HE21	2.16	0.58
1:B:164:ASP:OD2	1:B:166:HIS:CE1	2.57	0.58
1:B:614:ASN:HB3	1:B:626:GLY:CA	2.21	0.58
1:B:488:LEU:HD23	1:B:506:VAL:CG2	2.34	0.58
1:B:305:ARG:HD3	1:B:321:GLN:OE1	2.03	0.58
1:B:153:ASN:HD21	1:B:286:SER:HA	1.69	0.57
1:B:466:ARG:HG2	1:B:497:ASP:OD1	2.04	0.57
1:A:241:TYR:H	1:A:346:ARG:NH1	2.03	0.57
1:B:308:VAL:HG11	1:B:320:PHE:CZ	2.39	0.57
1:B:406:SER:O	1:B:407:VAL:HG23	2.04	0.57
1:A:269:GLU:CD	1:A:314:ASN:HD21	2.07	0.57
1:A:367:SER:HA	1:A:370:TRP:O	2.04	0.57
1:B:614:ASN:O	1:B:625:PHE:HD1	1.88	0.56
1:B:155:THR:HG23	1:B:167:GLN:HB3	1.86	0.56
1:B:220:TRP:HA	1:B:220:TRP:HE3	1.69	0.56
1:A:355:PRO:HG3	1:A:459:TYR:OH	2.04	0.56
1:A:493:GLN:N	1:A:501:THR:HG22	2.20	0.56
1:B:241:TYR:H	1:B:346:ARG:NH1	2.03	0.56
1:B:454:TYR:C	1:B:454:TYR:CD2	2.78	0.56
1:B:271:ASN:HD21	1:B:599:ASN:HD21	1.53	0.56
1:A:239:TRP:HD1	1:A:240:SER:O	1.89	0.56
1:B:422:ARG:O	1:B:423:LEU:HD23	2.06	0.56
1:A:267:ILE:HG22	1:A:268:ALA:N	2.21	0.56
1:A:386:ALA:CB	1:A:404:THR:HB	2.35	0.56
1:A:222:ALA:HB1	1:A:247:GLU:O	2.06	0.56
1:A:475:LEU:O	1:A:487:ASN:HA	2.06	0.56
1:B:155:THR:HG23	1:B:167:GLN:CB	2.35	0.55
1:B:379:ALA:HB3	1:B:382:TYR:HB3	1.88	0.55
1:B:498:ILE:HG13	1:B:499:ARG:N	2.19	0.55
1:B:233:SER:O	1:B:303:ARG:HG2	2.05	0.55
1:B:239:TRP:CZ2	1:B:357:PHE:CE1	2.89	0.55
1:B:212:TYR:N	1:B:212:TYR:CD2	2.75	0.55
1:A:236:PHE:CE2	1:A:377:VAL:HG23	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TYR:O	1:B:170:TYR:CG	2.57	0.55
1:B:602:TYR:HB3	1:B:613:ALA:HB3	1.87	0.55
1:B:150:TYR:CD1	1:B:150:TYR:C	2.80	0.55
1:A:408:ALA:HB1	1:A:454:TYR:HD1	1.71	0.55
1:A:565:ASN:N	1:A:565:ASN:HD22	2.05	0.55
1:A:343:GLY:O	1:A:357:PHE:CD2	2.59	0.55
1:A:409:ARG:HB3	1:A:415:THR:CG2	2.37	0.55
1:A:569:TYR:HE2	1:A:571:ASP:OD1	1.90	0.55
1:A:188:GLN:NE2	1:A:209:SER:HB3	2.22	0.54
1:A:484:THR:HA	1:A:509:ASN:O	2.08	0.54
1:A:277:SER:HA	1:A:283:LEU:HG	1.90	0.54
1:B:215:ARG:HD3	1:B:217:ILE:HD11	1.88	0.54
1:A:540:TYR:HE2	1:A:542:ARG:HB2	1.72	0.54
1:B:446:ARG:HA	1:B:496:TRP:NE1	2.22	0.54
1:A:566:MET:HE1	1:A:597:GLN:CG	2.36	0.54
1:B:525:SER:CB	1:B:540:TYR:HB3	2.37	0.54
1:A:178:LEU:O	1:A:181:TRP:HB2	2.08	0.54
1:A:235:ILE:HD12	1:A:361:GLU:HB2	1.90	0.54
1:B:577:LEU:O	1:B:578:ASP:OD1	2.25	0.54
1:A:563:TYR:HD2	1:A:565:ASN:HD21	1.49	0.54
1:B:503:TYR:HD1	1:B:529:SER:HA	1.72	0.54
1:B:456:ASN:C	1:B:458:ARG:H	2.10	0.54
1:A:327:VAL:HG13	1:A:328:PRO:HD2	1.90	0.54
1:B:325:ALA:HA	1:B:438:PHE:CD2	2.43	0.53
1:B:599:ASN:ND2	1:B:600:ALA:H	2.05	0.53
1:B:543:ILE:O	1:B:554:TYR:N	2.42	0.53
1:B:604:HIS:CE1	1:B:606:SER:HB2	2.43	0.53
1:A:205:ASN:HB3	1:B:199:GLU:HA	1.90	0.53
1:B:270:THR:HB	1:B:313:GLN:OE1	2.08	0.53
1:B:466:ARG:HB2	1:B:497:ASP:OD1	2.09	0.53
1:A:159:ASN:HD22	1:A:163:GLY:N	2.07	0.53
1:A:271:ASN:N	1:A:290:ALA:HB2	2.24	0.53
1:B:178:LEU:O	1:B:180:PRO:N	2.42	0.53
1:B:622:TYR:CD1	1:B:622:TYR:C	2.82	0.53
1:A:385:LEU:O	1:A:404:THR:HA	2.09	0.52
1:A:427:LYS:HB3	1:A:437:THR:HG23	1.91	0.52
1:B:213:LEU:HB2	1:B:226:LEU:HD21	1.91	0.52
1:B:265:THR:HB	1:B:293:PHE:O	2.09	0.52
1:B:173:THR:HA	1:B:185:ALA:O	2.09	0.52
1:A:336:VAL:CG2	1:A:364:TRP:HA	2.39	0.52
1:A:446:ARG:CA	1:A:496:TRP:HE1	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:HD2	1:B:229:ASN:HD22	1.74	0.52
1:B:239:TRP:CZ2	1:B:357:PHE:HE1	2.24	0.52
1:A:356:VAL:HG12	1:A:357:PHE:H	1.72	0.52
1:B:271:ASN:ND2	1:B:614:ASN:OD1	2.36	0.52
1:A:570:THR:CB	1:A:581:SER:HB3	2.25	0.52
1:A:454:TYR:C	1:A:454:TYR:CD2	2.83	0.52
1:B:278:GLN:NE2	1:B:306:LEU:CD2	2.73	0.52
1:A:336:VAL:HG23	1:A:364:TRP:HA	1.92	0.52
1:B:583:ASN:N	1:B:583:ASN:HD22	2.07	0.52
1:A:416:PHE:HB3	1:A:447:ASN:HB3	1.91	0.52
1:B:567:ALA:O	1:B:583:ASN:HA	2.09	0.52
1:B:182:ARG:NH2	1:B:216:ALA:H	2.08	0.52
1:B:467:GLU:HG2	1:B:493:GLN:OE1	2.10	0.52
1:B:264:ILE:HD12	1:B:298:LEU:HD11	1.92	0.51
1:B:369:GLN:O	1:B:391:TRP:HA	2.10	0.51
1:A:425:TYR:O	1:A:438:PHE:HA	2.10	0.51
1:B:506:VAL:O	1:B:526:ALA:HB3	2.09	0.51
1:A:150:TYR:CE1	1:A:630:SER:HA	2.45	0.51
1:B:273:ARG:HA	1:B:286:SER:O	2.11	0.51
1:B:622:TYR:HD1	1:B:623:THR:O	1.92	0.51
1:B:228:GLU:HG2	1:B:346:ARG:NE	2.26	0.51
1:B:599:ASN:HD22	1:B:600:ALA:H	1.59	0.51
1:A:416:PHE:N	1:A:416:PHE:CD1	2.79	0.51
1:A:496:TRP:HA	1:A:496:TRP:CE3	2.45	0.51
1:A:573:PHE:HE1	1:A:578:ASP:OD2	1.94	0.51
1:B:303:ARG:NH1	1:B:422:ARG:NH2	2.59	0.51
1:B:457:ALA:HA	1:B:462:ASP:H	1.72	0.50
1:A:398:THR:HG22	1:A:399:LEU:H	1.75	0.50
1:A:496:TRP:HA	1:A:496:TRP:HE3	1.77	0.50
1:B:579:SER:HB3	1:B:603:SER:OG	2.11	0.50
1:B:611:LEU:HA	1:B:628:SER:O	2.12	0.50
1:A:269:GLU:OE2	1:A:314:ASN:ND2	2.43	0.50
1:A:470:MET:HE1	1:A:472:THR:HB	1.93	0.50
1:A:182:ARG:HH22	1:A:216:ALA:HB3	1.77	0.50
1:A:232:ASN:HB2	1:A:303:ARG:HG2	1.93	0.50
1:A:441:TYR:OH	1:A:469:GLU:HG2	2.11	0.50
1:B:152:LEU:HB2	1:B:629:ALA:HB3	1.94	0.50
1:B:456:ASN:O	1:B:458:ARG:N	2.44	0.50
1:A:381:ASP:HB3	1:A:409:ARG:O	2.11	0.50
1:B:579:SER:HB3	1:B:603:SER:HG	1.76	0.50
1:A:399:LEU:HA	1:A:424:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:HB	1:A:475:LEU:CD2	2.40	0.49
1:B:271:ASN:HB2	1:B:614:ASN:HD21	1.77	0.49
1:B:494:THR:HG22	1:B:500:LYS:HB2	1.94	0.49
1:A:483:ASN:O	1:A:484:THR:HB	2.11	0.49
1:B:213:LEU:HB2	1:B:226:LEU:CD2	2.43	0.49
1:B:239:TRP:CD1	1:B:240:SER:O	2.66	0.49
1:B:406:SER:O	1:B:407:VAL:CG2	2.60	0.49
1:B:536:ASN:OD1	1:B:537:ASP:N	2.45	0.49
1:A:159:ASN:HD22	1:A:163:GLY:H	1.59	0.49
1:A:331:THR:HG22	1:A:332:ARG:N	2.28	0.49
1:A:410:ILE:HG23	1:A:458:ARG:HG3	1.93	0.49
1:B:206:PHE:CD1	1:B:207:THR:N	2.80	0.49
1:B:265:THR:O	1:B:505:THR:HG21	2.11	0.49
1:B:266:GLY:O	1:B:267:ILE:HG12	2.12	0.49
1:B:525:SER:HB2	1:B:540:TYR:HB3	1.94	0.49
1:B:422:ARG:HA	1:B:441:TYR:O	2.12	0.49
1:B:236:PHE:CE1	1:B:377:VAL:HG22	2.48	0.49
1:B:312:GLU:OE1	1:B:312:GLU:HA	2.13	0.49
1:B:420:SER:HA	1:B:443:PHE:O	2.13	0.49
1:B:231:ILE:HG21	1:B:239:TRP:CZ3	2.49	0.48
1:B:305:ARG:HA	1:B:323:ASP:HA	1.95	0.48
1:B:406:SER:HG	1:B:448:TYR:HD1	1.58	0.48
1:A:150:TYR:O	1:A:150:TYR:CD1	2.66	0.48
1:A:302:VAL:HG12	1:A:324:THR:HG21	1.96	0.48
1:B:386:ALA:HB2	1:B:404:THR:HB	1.95	0.48
1:A:520:VAL:HG12	1:A:521:ALA:N	2.28	0.48
1:B:463:TYR:HB3	1:B:466:ARG:HH21	1.78	0.48
1:A:338:TYR:CD1	1:A:338:TYR:C	2.87	0.48
1:A:150:TYR:CD1	1:A:150:TYR:C	2.87	0.48
1:A:562:ARG:O	1:A:562:ARG:HG2	2.13	0.48
1:A:563:TYR:CD2	1:A:565:ASN:ND2	2.78	0.48
1:B:217:ILE:O	1:B:220:TRP:O	2.32	0.48
1:B:181:TRP:CE2	1:B:215:ARG:HD2	2.49	0.48
1:B:472:THR:HA	1:B:490:TYR:O	2.14	0.48
1:A:450:THR:O	1:A:453:GLN:N	2.47	0.48
1:A:613:ALA:HA	1:A:626:GLY:O	2.14	0.47
1:B:271:ASN:ND2	1:B:599:ASN:HD21	2.12	0.47
1:A:493:GLN:HE21	1:A:493:GLN:HA	1.80	0.47
1:A:159:ASN:HB3	1:A:163:GLY:N	2.27	0.47
1:A:271:ASN:HD21	1:A:599:ASN:HD21	1.57	0.47
1:A:451:MET:HE1	1:A:455:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:CG1	1:A:357:PHE:H	2.28	0.47
1:B:253:LEU:HG	1:B:254:PRO:HD2	1.97	0.47
1:A:372:LEU:HA	1:A:389:ALA:HA	1.97	0.47
1:A:446:ARG:HA	1:A:496:TRP:CD1	2.50	0.47
1:A:595:GLN:HB2	1:A:618:LEU:HD22	1.96	0.47
1:B:454:TYR:O	1:B:458:ARG:HB2	2.14	0.47
1:B:495:TYR:CD1	1:B:498:ILE:HG12	2.50	0.47
1:A:278:GLN:NE2	1:A:305:ARG:O	2.40	0.47
1:B:599:ASN:ND2	1:B:600:ALA:N	2.63	0.47
1:A:356:VAL:CG1	1:A:357:PHE:N	2.78	0.47
1:B:278:GLN:OE1	1:B:304:GLY:HA3	2.15	0.47
1:A:490:TYR:HD1	1:A:504:TYR:HB2	1.79	0.47
1:B:523:GLY:HA3	1:B:542:ARG:HB3	1.96	0.47
1:B:271:ASN:HB2	1:B:614:ASN:ND2	2.30	0.46
1:B:488:LEU:HD13	1:B:488:LEU:O	2.14	0.46
1:A:183:LEU:HG	1:A:213:LEU:HD21	1.97	0.46
1:B:155:THR:CG2	1:B:167:GLN:HB3	2.45	0.46
1:B:206:PHE:CD1	1:B:206:PHE:C	2.88	0.46
1:B:339:LYS:O	1:B:340:LEU:HD23	2.16	0.46
1:A:188:GLN:HG2	1:A:207:THR:CG2	2.46	0.46
1:B:377:VAL:O	1:B:378:LEU:HD23	2.15	0.46
1:B:451:MET:O	1:B:455:LEU:HG	2.15	0.46
1:B:503:TYR:CD1	1:B:528:ARG:O	2.68	0.46
1:A:264:ILE:HD11	1:A:306:LEU:HD13	1.98	0.46
1:B:172:GLY:O	1:B:186:ASP:HA	2.16	0.46
1:A:408:ALA:HB3	1:A:449:MET:CE	2.46	0.46
1:B:167:GLN:OE1	1:B:168:PHE:N	2.49	0.46
1:B:502:ASP:OD2	1:B:528:ARG:HD3	2.15	0.46
1:B:602:TYR:OH	1:B:604:HIS:HB2	2.16	0.46
1:B:604:HIS:O	1:B:604:HIS:CG	2.69	0.46
1:A:305:ARG:HA	1:A:323:ASP:HA	1.97	0.46
1:A:320:PHE:HB2	1:A:503:TYR:CD1	2.50	0.46
1:B:231:ILE:O	1:B:231:ILE:HG22	2.16	0.46
1:A:179:GLY:HA3	1:A:180:PRO:HD3	1.77	0.45
1:A:187:TYR:O	1:A:187:TYR:CG	2.68	0.45
1:A:235:ILE:HD12	1:A:361:GLU:CB	2.46	0.45
1:B:192:GLU:OE2	1:B:192:GLU:N	2.48	0.45
1:B:405:GLN:HA	1:B:419:LYS:HA	1.97	0.45
1:A:194:SER:C	1:A:195:ARG:HG2	2.37	0.45
1:B:181:TRP:CZ2	1:B:215:ARG:HD2	2.52	0.45
1:B:381:ASP:OD1	1:B:409:ARG:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG22	1:A:241:TYR:CE2	2.52	0.45
1:A:332:ARG:CG	1:A:332:ARG:NH1	2.58	0.45
1:B:303:ARG:CZ	1:B:326:SER:HB2	2.47	0.45
1:B:252:MET:SD	1:B:253:LEU:HB2	2.56	0.45
1:A:239:TRP:CD1	1:A:240:SER:O	2.70	0.45
1:A:267:ILE:CG2	1:A:268:ALA:N	2.80	0.45
1:A:169:SER:O	1:A:170:TYR:HB3	2.17	0.45
1:A:488:LEU:O	1:A:488:LEU:HD13	2.17	0.45
1:B:270:THR:OG1	1:B:312:GLU:OE1	2.30	0.45
1:A:201:THR:O	1:A:202:THR:HG22	2.17	0.45
1:A:231:ILE:HG22	1:A:241:TYR:CD2	2.52	0.45
1:A:522:VAL:HG22	1:A:543:ILE:HG13	1.98	0.45
1:B:231:ILE:CD1	1:B:341:VAL:HG11	2.43	0.45
1:B:288:VAL:HG11	1:B:293:PHE:CB	2.46	0.45
1:A:170:TYR:CD2	1:A:170:TYR:C	2.89	0.45
1:A:403:ILE:CD1	1:A:421:TRP:CD1	2.93	0.45
1:A:403:ILE:CD1	1:A:421:TRP:HD1	2.28	0.45
1:B:329:TYR:CE1	1:B:363:SER:HB2	2.52	0.45
1:A:147:MET:CG	1:A:633:ALA:O	2.62	0.45
1:A:635:ILE:O	1:A:636:THR:HB	2.16	0.45
1:B:450:THR:H	1:B:453:GLN:HB2	1.82	0.45
1:A:610:ASN:N	1:A:630:SER:O	2.49	0.44
1:A:488:LEU:HD13	1:A:488:LEU:C	2.36	0.44
1:B:170:TYR:CZ	1:B:189:GLY:HA3	2.53	0.44
1:B:614:ASN:O	1:B:625:PHE:CD1	2.69	0.44
1:A:235:ILE:CD1	1:A:361:GLU:HB2	2.47	0.44
1:A:273:ARG:NH2	1:A:311:ILE:HD13	2.31	0.44
1:A:287:MET:CE	1:A:601:TYR:CE1	3.01	0.44
1:A:401:ALA:HA	1:A:422:ARG:O	2.17	0.44
1:B:449:MET:HA	1:B:453:GLN:OE1	2.18	0.44
1:B:501:THR:OG1	1:B:530:LYS:HG3	2.17	0.44
1:B:231:ILE:HG21	1:B:239:TRP:CE3	2.52	0.44
1:B:608:LEU:HD22	1:B:608:LEU:HA	1.77	0.44
1:A:384:ALA:HA	1:A:405:GLN:O	2.17	0.44
1:B:455:LEU:HD23	1:B:455:LEU:HA	1.84	0.44
1:A:206:PHE:CG	1:A:207:THR:N	2.85	0.43
1:B:337:ARG:H	1:B:337:ARG:HG3	1.63	0.43
1:A:336:VAL:HG22	1:A:363:SER:O	2.18	0.43
1:A:615:ILE:HG12	1:A:625:PHE:HD1	1.82	0.43
1:B:222:ALA:HB1	1:B:247:GLU:O	2.17	0.43
1:B:490:TYR:HD1	1:B:504:TYR:CB	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:C	1:A:370:TRP:O	2.57	0.43
1:A:369:GLN:O	1:A:391:TRP:HA	2.19	0.43
1:A:622:TYR:CD1	1:A:622:TYR:C	2.92	0.43
1:B:321:GLN:O	1:B:322:VAL:HG22	2.18	0.43
1:B:332:ARG:O	1:B:335:GLN:N	2.47	0.43
1:A:445:GLU:O	1:A:446:ARG:C	2.56	0.43
1:A:457:ALA:HA	1:A:462:ASP:O	2.18	0.43
1:A:563:TYR:CE2	1:A:565:ASN:ND2	2.83	0.43
1:B:583:ASN:O	1:B:584:ALA:HB2	2.19	0.43
1:A:270:THR:O	1:A:272:ALA:N	2.47	0.43
1:A:306:LEU:HD11	1:A:324:THR:HG22	1.99	0.43
1:A:365:GLY:HA2	1:A:371:SER:HB3	2.00	0.43
1:B:249:ASP:O	1:B:252:MET:SD	2.76	0.43
1:B:528:ARG:HB2	1:B:537:ASP:OD1	2.18	0.43
1:A:178:LEU:HA	1:A:178:LEU:HD12	1.65	0.43
1:A:232:ASN:HB2	1:A:303:ARG:CG	2.48	0.43
1:A:238:SER:OG	1:A:239:TRP:N	2.51	0.43
1:A:395:VAL:N	1:A:396:PRO:CD	2.80	0.43
1:A:422:ARG:HA	1:A:441:TYR:O	2.19	0.43
1:B:457:ALA:HB2	1:B:463:TYR:HA	2.01	0.43
1:A:270:THR:N	1:A:312:GLU:OE1	2.51	0.43
1:B:470:MET:HG2	1:B:471:TYR:N	2.31	0.43
1:A:267:ILE:HD13	1:A:540:TYR:CB	2.49	0.43
1:A:285:ASP:CG	1:A:285:ASP:O	2.54	0.43
1:A:511:TYR:O	1:A:512:PHE:C	2.57	0.43
1:A:540:TYR:CE2	1:A:542:ARG:HB2	2.52	0.43
1:B:345:SER:OG	1:B:355:PRO:HD2	2.19	0.43
1:A:194:SER:HB2	1:A:201:THR:HG23	2.01	0.43
1:A:269:GLU:N	1:A:312:GLU:OE2	2.52	0.43
1:A:273:ARG:NH2	1:A:311:ILE:CD1	2.82	0.43
1:B:212:TYR:N	1:B:212:TYR:HD2	2.17	0.43
1:B:240:SER:O	1:B:241:TYR:HB3	2.19	0.43
1:B:344:ARG:HH21	1:B:356:VAL:CG2	2.32	0.43
1:A:466:ARG:HA	1:A:466:ARG:HD2	1.58	0.42
1:B:493:GLN:HE21	1:B:493:GLN:C	2.22	0.42
1:A:237:ARG:HH12	1:A:442:ARG:NH1	2.17	0.42
1:A:313:GLN:NE2	1:A:624:SER:OG	2.53	0.42
1:B:239:TRP:HD1	1:B:240:SER:O	2.03	0.42
1:A:388:GLY:HA3	1:A:402:ASP:HB3	2.00	0.42
1:B:278:GLN:NE2	1:B:306:LEU:HD21	2.34	0.42
1:B:409:ARG:HB3	1:B:415:THR:CG2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:THR:HA	1:B:527:SER:HA	2.00	0.42
1:A:611:LEU:C	1:A:611:LEU:HD23	2.40	0.42
1:B:278:GLN:HB2	1:B:306:LEU:HD22	2.02	0.42
1:B:288:VAL:HG11	1:B:293:PHE:HB3	2.02	0.42
1:A:153:ASN:OD1	1:A:286:SER:HA	2.19	0.42
1:A:186:ASP:HB2	1:A:210:ARG:H	1.84	0.42
1:A:449:MET:CG	1:A:466:ARG:HH22	2.20	0.42
1:B:303:ARG:NH1	1:B:422:ARG:HH22	2.17	0.42
1:A:146:LEU:HD23	1:A:635:ILE:HB	2.01	0.42
1:A:184:ARG:HH21	1:A:214:PHE:HE2	1.68	0.42
1:A:520:VAL:CG1	1:A:521:ALA:N	2.83	0.42
1:A:565:ASN:N	1:A:565:ASN:ND2	2.65	0.42
1:B:525:SER:HB2	1:B:540:TYR:CB	2.50	0.42
1:B:204:ARG:O	1:B:205:ASN:HB3	2.20	0.42
1:B:235:ILE:HA	1:B:422:ARG:NH1	2.32	0.42
1:B:323:ASP:OD1	1:B:323:ASP:N	2.51	0.42
1:A:488:LEU:HD22	1:A:489:GLN:N	2.35	0.42
1:B:522:VAL:HG12	1:B:523:GLY:N	2.32	0.42
1:A:419:LYS:HB3	1:A:419:LYS:HE3	1.80	0.41
1:A:470:MET:HA	1:A:492:ARG:O	2.19	0.41
1:B:305:ARG:HD3	1:B:321:GLN:NE2	2.35	0.41
1:B:490:TYR:HD1	1:B:504:TYR:CD1	2.38	0.41
1:A:449:MET:HG3	1:A:466:ARG:NH2	2.18	0.41
1:B:456:ASN:C	1:B:458:ARG:N	2.72	0.41
1:B:622:TYR:HD1	1:B:623:THR:N	2.18	0.41
1:A:289:PRO:O	1:A:290:ALA:C	2.57	0.41
1:A:528:ARG:HB3	1:A:537:ASP:OD1	2.20	0.41
1:A:305:ARG:HG3	1:A:306:LEU:N	2.36	0.41
1:B:181:TRP:CE3	1:B:215:ARG:HB3	2.56	0.41
1:B:187:TYR:O	1:B:187:TYR:CG	2.73	0.41
1:B:228:GLU:HG2	1:B:346:ARG:CD	2.50	0.41
1:B:233:SER:OG	1:B:234:ASP:N	2.52	0.41
1:B:450:THR:O	1:B:451:MET:C	2.59	0.41
1:A:367:SER:CA	1:A:370:TRP:O	2.69	0.41
1:A:451:MET:O	1:A:455:LEU:HG	2.21	0.41
1:B:203:ASN:OD1	1:B:203:ASN:C	2.59	0.41
1:B:391:TRP:CD1	1:B:391:TRP:C	2.94	0.41
1:B:228:GLU:HG2	1:B:346:ARG:HD2	2.03	0.41
1:B:274:VAL:O	1:B:285:ASP:HA	2.21	0.41
1:A:269:GLU:HB3	1:A:312:GLU:OE2	2.21	0.41
1:A:312:GLU:HB2	1:A:316:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ASN:HA	1:A:522:VAL:O	2.20	0.41
1:A:619:GLN:HG2	1:A:620:LYS:N	2.36	0.41
1:B:187:TYR:HB3	1:B:208:TRP:CE3	2.56	0.41
1:B:232:ASN:OD1	1:B:232:ASN:C	2.59	0.41
1:A:207:THR:OG1	1:A:208:TRP:N	2.53	0.41
1:A:420:SER:HB3	1:A:444:SER:HA	2.03	0.41
1:A:536:ASN:CG	1:A:537:ASP:N	2.75	0.41
1:B:466:ARG:HB2	1:B:496:TRP:HB2	2.02	0.41
1:A:151:ASN:O	1:A:170:TYR:HA	2.21	0.40
1:A:190:SER:O	1:A:190:SER:OG	2.32	0.40
1:A:357:PHE:HB2	1:A:378:LEU:O	2.22	0.40
1:B:406:SER:OG	1:B:448:TYR:HD1	2.03	0.40
1:B:622:TYR:CD1	1:B:623:THR:N	2.89	0.40
1:B:629:ALA:O	1:B:630:SER:HB3	2.21	0.40
1:A:233:SER:OG	1:A:361:GLU:OE2	2.29	0.40
1:A:267:ILE:HD13	1:A:540:TYR:HB2	2.04	0.40
1:A:501:THR:O	1:A:501:THR:CG2	2.69	0.40
1:A:596:ARG:O	1:A:618:LEU:HD23	2.21	0.40
1:A:635:ILE:O	1:A:636:THR:CB	2.69	0.40
1:B:451:MET:HE3	1:B:455:LEU:HG	2.02	0.40
1:B:526:ALA:O	1:B:527:SER:HB3	2.22	0.40
1:A:362:ALA:O	1:A:373:TYR:HB2	2.22	0.40
1:B:241:TYR:H	1:B:346:ARG:HH11	1.70	0.40
1:B:155:THR:HG23	1:B:167:GLN:HB2	2.02	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	408/493 (83%)	349 (86%)	53 (13%)	6 (2%)	10 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	338/493 (69%)	262 (78%)	67 (20%)	9 (3%)	5 27
All	All	746/986 (76%)	611 (82%)	120 (16%)	15 (2%)	7 34

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	TYR
1	B	457	ALA
1	A	333	PRO
1	A	451	MET
1	B	221	ARG
1	B	262	PRO
1	B	267	ILE
1	B	411	GLU
1	A	458	ARG
1	A	218	PRO
1	A	271	ASN
1	A	446	ARG
1	B	451	MET
1	B	407	VAL
1	B	218	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	351/405 (87%)	273 (78%)	78 (22%)	1 4
1	B	292/405 (72%)	218 (75%)	74 (25%)	0 2
All	All	643/810 (79%)	491 (76%)	152 (24%)	1 3

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	153	ASN
1	A	155	THR
1	A	158	ARG
1	A	161	GLN
1	A	178	LEU
1	A	191	GLN
1	A	201	THR
1	A	204	ARG
1	A	211	PHE
1	A	214	PHE
1	A	215	ARG
1	A	219	ARG
1	A	223	ASN
1	A	225	THR
1	A	226	LEU
1	A	229	ASN
1	A	230	ASN
1	A	231	ILE
1	A	249	ASP
1	A	273	ARG
1	A	278	GLN
1	A	294	SER
1	A	296	GLN
1	A	297	ASP
1	A	305	ARG
1	A	323	ASP
1	A	324	THR
1	A	329	TYR
1	A	332	ARG
1	A	336	VAL
1	A	337	ARG
1	A	346	ARG
1	A	366	LEU
1	A	368	ASN
1	A	369	GLN
1	A	371	SER
1	A	372	LEU
1	A	385	LEU
1	A	393	LEU
1	A	404	THR
1	A	411	GLU
1	A	415	THR

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Mol	Chain	Res	Type
1	A	417	GLN
1	A	419	LYS
1	A	437	THR
1	A	451	MET
1	A	454	TYR
1	A	466	ARG
1	A	472	THR
1	A	486	PHE
1	A	488	LEU
1	A	493	GLN
1	A	496	TRP
1	A	498	ILE
1	A	501	THR
1	A	504	TYR
1	A	505	THR
1	A	507	SER
1	A	511	TYR
1	A	528	ARG
1	A	547	LEU
1	A	557	SER
1	A	559	SER
1	A	565	ASN
1	A	570	THR
1	A	574	ASN
1	A	578	ASP
1	A	581	SER
1	A	594	SER
1	A	595	GLN
1	A	614	ASN
1	A	615	ILE
1	A	617	SER
1	A	618	LEU
1	A	623	THR
1	A	635	ILE
1	A	636	THR
1	B	148	LEU
1	B	151	ASN
1	B	152	LEU
1	B	158	ARG
1	B	169	SER
1	B	173	THR
1	B	186	ASP

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Mol	Chain	Res	Type
1	B	201	THR
1	B	204	ARG
1	B	212	TYR
1	B	214	PHE
1	B	219	ARG
1	B	220	TRP
1	B	221	ARG
1	B	224	LEU
1	B	225	THR
1	B	229	ASN
1	B	231	ILE
1	B	235	ILE
1	B	237	ARG
1	B	242	THR
1	B	246	LEU
1	B	252	MET
1	B	265	THR
1	B	296	GLN
1	B	302	VAL
1	B	303	ARG
1	B	319	THR
1	B	329	TYR
1	B	337	ARG
1	B	340	LEU
1	B	341	VAL
1	B	342	SER
1	B	344	ARG
1	B	345	SER
1	B	346	ARG
1	B	361	GLU
1	B	371	SER
1	B	391	TRP
1	B	393	LEU
1	B	398	THR
1	B	400	SER
1	B	403	ILE
1	B	404	THR
1	B	409	ARG
1	B	416	PHE
1	B	420	SER
1	B	451	MET
1	B	454	TYR

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Mol	Chain	Res	Type
1	B	458	ARG
1	B	463	TYR
1	B	470	MET
1	B	493	GLN
1	B	497	ASP
1	B	498	ILE
1	B	500	LYS
1	B	504	TYR
1	B	508	VAL
1	B	524	LEU
1	B	530	LYS
1	B	535	ASP
1	B	538	SER
1	B	542	ARG
1	B	543	ILE
1	B	566	MET
1	B	577	LEU
1	B	581	SER
1	B	583	ASN
1	B	604	HIS
1	B	608	LEU
1	B	617	SER
1	B	618	LEU
1	B	622	TYR
1	B	623	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	153	ASN
1	A	159	ASN
1	A	161	GLN
1	A	166	HIS
1	A	229	ASN
1	A	313	GLN
1	A	369	GLN
1	A	417	GLN
1	A	493	GLN
1	A	565	ASN
1	A	587	ASN
1	A	595	GLN

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Mol	Chain	Res	Type
1	A	597	GLN
1	A	599	ASN
1	B	151	ASN
1	B	153	ASN
1	B	166	HIS
1	B	229	ASN
1	B	278	GLN
1	B	447	ASN
1	B	493	GLN
1	B	583	ASN
1	B	599	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	436/493 (88%)	0.17	11 (2%)	57	42	86, 114, 136, 158	11 (2%)
1	B	384/493 (77%)	0.26	24 (6%)	20	10	97, 126, 155, 171	4 (1%)
All	All	820/986 (83%)	0.21	35 (4%)	35	21	86, 120, 150, 171	15 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	LEU	6.1
1	A	503	TYR	5.1
1	B	324	THR	5.1
1	B	325	ALA	4.8
1	B	361	GLU	3.5
1	B	322	VAL	3.5
1	B	503	TYR	3.5
1	B	323	ASP	3.5
1	B	633	ALA	3.4
1	B	267	ILE	3.2
1	B	391	TRP	3.2
1	B	213	LEU	3.1
1	B	272	ALA	2.9
1	A	348	TYR	2.9
1	B	212	TYR	2.8
1	B	635	ILE	2.8
1	B	564	VAL	2.6
1	A	302	VAL	2.6
1	B	269	GLU	2.6
1	A	308	VAL	2.6
1	A	322	VAL	2.4
1	B	298	LEU	2.4
1	B	580	TYR	2.3
1	A	562	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	443	PHE	2.3
1	B	306	LEU	2.3
1	B	624	SER	2.2
1	B	393	LEU	2.1
1	B	339	LYS	2.1
1	B	632	GLY	2.1
1	A	486	PHE	2.1
1	A	502	ASP	2.1
1	B	438	PHE	2.0
1	A	174	VAL	2.0
1	A	489	GLN	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.