Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 03:05 AM EDT

PDB ID	:	3UA4
Title	:	Crystal Structure of Protein Arginine Methyltransferase PRMT5
Authors	:	Sun, L.; Wang, M.; Lv, Z.; Yang, N.; Liu, Y.; Bao, S.; Gong, W.; Xu, R.M.
Deposited on	:	2011-10-21
Resolution	:	3.00 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

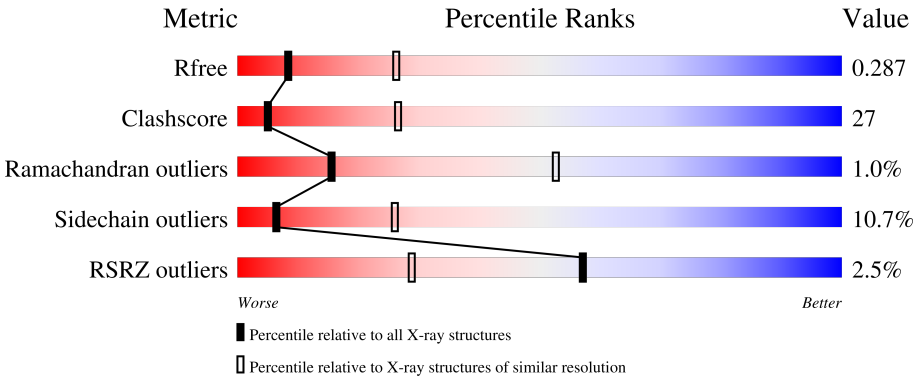
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	745	2% 45% 37% · 14%
1	B	745	3% 41% 38% 6% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10345 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.

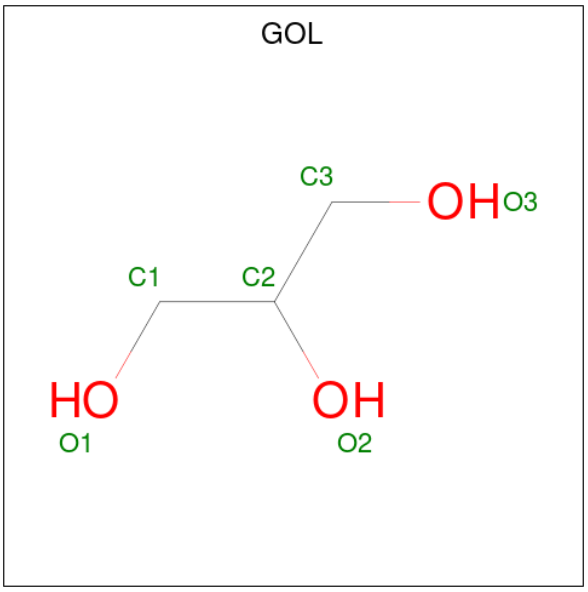
- Molecule 1 is a protein called Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			5143	3291	875	957	20			
1	B	628	Total	C	N	O	S	1	0	0
			5049	3238	854	937	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P46580
A	-1	ALA	-	expression tag	UNP P46580
A	0	SER	-	expression tag	UNP P46580
A	735	LEU	-	expression tag	UNP P46580
A	736	GLU	-	expression tag	UNP P46580
A	737	HIS	-	expression tag	UNP P46580
A	738	HIS	-	expression tag	UNP P46580
A	739	HIS	-	expression tag	UNP P46580
A	740	HIS	-	expression tag	UNP P46580
A	741	HIS	-	expression tag	UNP P46580
A	742	HIS	-	expression tag	UNP P46580
B	-2	MET	-	expression tag	UNP P46580
B	-1	ALA	-	expression tag	UNP P46580
B	0	SER	-	expression tag	UNP P46580
B	735	LEU	-	expression tag	UNP P46580
B	736	GLU	-	expression tag	UNP P46580
B	737	HIS	-	expression tag	UNP P46580
B	738	HIS	-	expression tag	UNP P46580
B	739	HIS	-	expression tag	UNP P46580
B	740	HIS	-	expression tag	UNP P46580
B	741	HIS	-	expression tag	UNP P46580
B	742	HIS	-	expression tag	UNP P46580

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

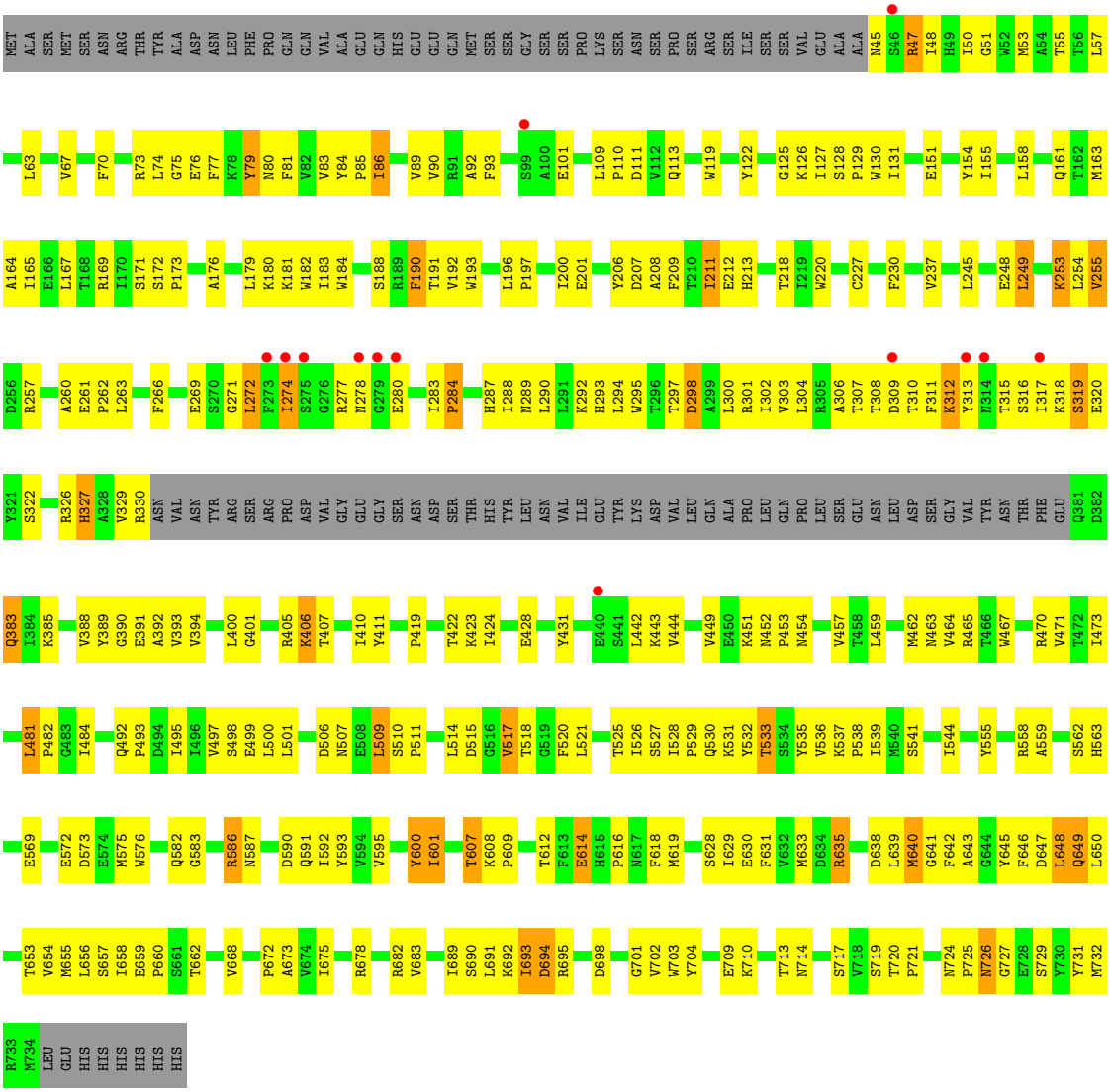
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	74	Total O 74 74	0	0
3	B	73	Total O 73 73	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein arginine N-methyltransferase 5

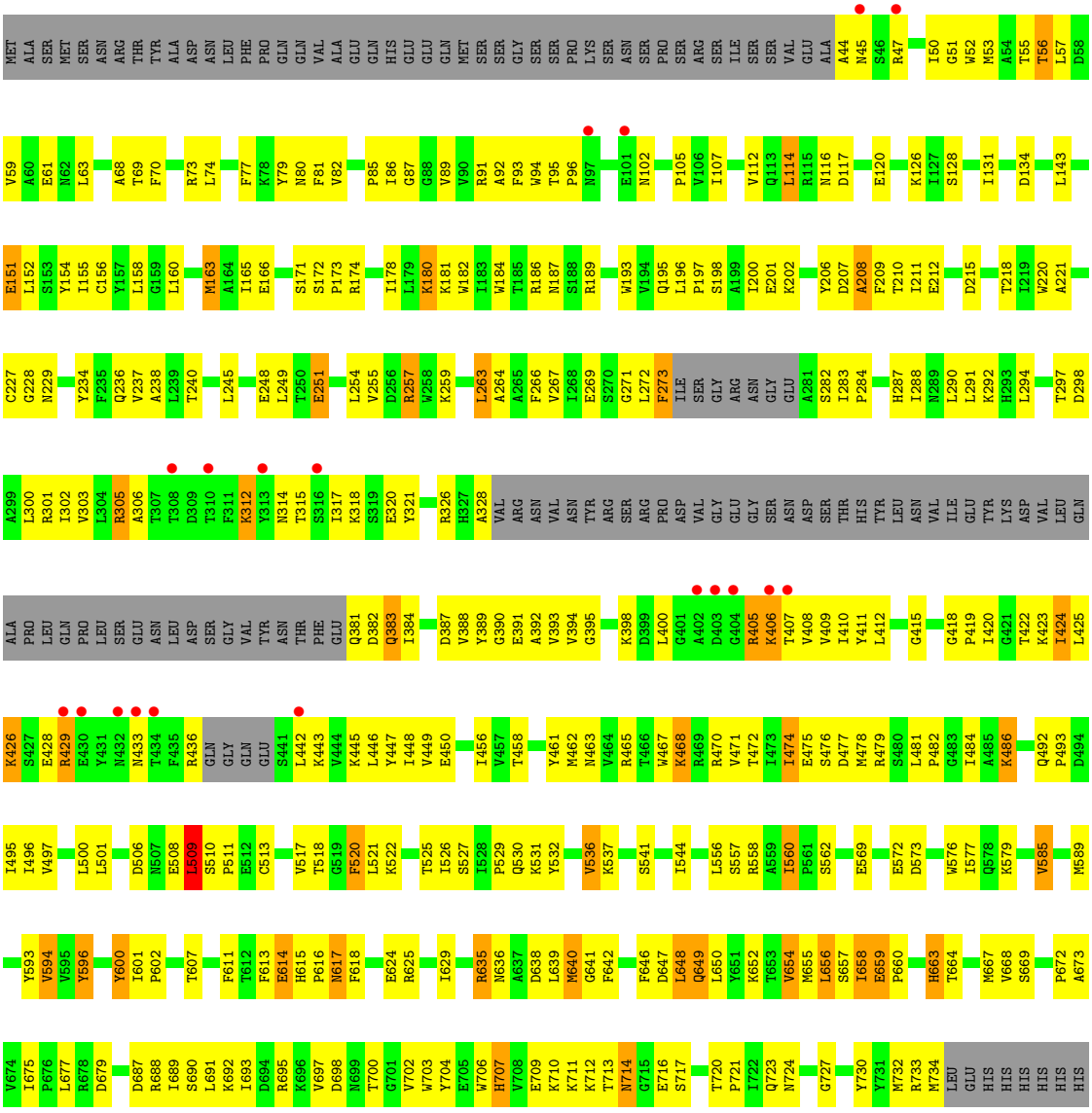
Chain A:



• Molecule 1: Protein arginine N-methyltransferase 5

Chain B:


3%
41%
38%
6%
16%


MET ALA SER MET SER ASN ARG THR TYR ALA ASP ASN LEU PHE PRO GLN GLN VAL ALA GLU GLN HIS GLU GLU GLN MET SER SER GLY SER SER PRO LYS SER ASN SER PRO SER ARG SER ILE SER SER VAL GLU ALA A44 N45 S46 R47 I50 G51 W52 M53 A54 T55 T56 L57 D58
V59 A60 E61 N62 L63 A68 T69 F70 R73 L74 F77 K78 Y79 N80 F81 V82 P85 I86 G87 G88 V89 V90 R91 A92 F93 W94 T95 P96 N97 E101 N102 P105 V106 I107 V112 Q113 L114 R115 N116 D117 E120 K126 I127 S128 I131 D134 L143
E151 L152 S153 Y154 I155 C156 Y157 L158 G159 L160 M163 A164 I165 E166 S171 S172 P173 R174 I178 L179 K180 K181 W182 I183 W184 T185 R186 N187 S188 R189 W193 V194 Q195 L196 P197 S198 A199 I200 E201 K202 Y206 D207 A208 F209 T210 I211 E212 D215 T218 I219 W220 A221
C227 G228 N229 Y234 F235 Q236 V237 A238 L239 T240 L245 E248 L249 T250 E251 L254 V255 D256 R267 W258 K259 L263 A264 A265 F266 V267 I268 E269 S270 G271 L272 F273 ILE SER GLY ARG ASN GLY GLU A281 S282 I283 P284 H287 I288 N289 L290 L291 K292 H293 L294 T297 D298
A299 L300 R301 I302 V303 L304 R305 A306 T307 T308 D309 T310 F311 K312 Y313 N314 T315 S316 I317 K318 S319 E320 Y321 R326 H327 A328 VAL ARG ASN VAL ASN TYR ARG SER ARG PRO ASP VAL GLY GLU GLY SER ASN ASP SER THR HIS TYR LEU ASN VAL ILE GLU TYR LYS ASP VAL LEU GLN
ALA PRO LEU GLN PRO LEU SER GLU ASN LEU ASP SER GLY VAL TYR ASN THR PHE GLU Q381 D382 Q383 I384 D387 V388 Y389 G390 E391 A392 V393 V394 G395 K398 D399 L400 G401 A402 D403 G404 R405 K406 T407 V408 V409 I410 Y411 L412 G415 G418 P419 I420 G421 T422 K423 I424 L425
K426 S427 E428 R429 E430 Y431 N432 N433 T434 F435 R436 GLN GLY GLN GLU S441 L442 K443 V444 K445 L446 Y447 I448 V449 E450 I456 V457 T458 Y461 M462 N463 V464 R465 T466 W467 K468 R469 R470 V471 T472 I473 I474 E475 S476 D477 M478 R479 S480 L481 P482 G483 I484 A485 K486 Q492 P493 D494
I495 I496 V497 L500 L501 D506 N507 E508 L509 S510 P511 E512 C513 V517 T518 G519 P520 L521 K522 T525 I526 S527 I528 P529 Q530 K531 Y532 V536 K537 S541 I544 L556 S557 R558 A559 I560 P561 S562 E569 E572 D573 W576 I577 Q578 K579 V585 M589
Y593 V594 V595 Y596 Y600 I601 P602 T607 F611 T612 F613 E614 H615 P616 N617 F618 E624 R625 I629 R635 N636 A637 D638 L639 M640 G641 F642 F646 D647 L648 Q649 L650 Y651 K652 T653 V654 M655 L656 S657 I658 E659 P660 H663 T664 M667 V668 S669 P672 A673
V674 I675 P676 L677 R678 D679 D687 R688 I689 S690 L691 K692 I693 D694 R695 K696 V697 D698 N699 T700 G701 V702 W703 Y704 E705 W706 H707 V708 E709 K710 K711 K712 T713 N714 G715 E716 S717 T720 P721 I722 Q723 N724 G727 Y730 Y731 M732 R733 M734 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.56Å 129.49Å 149.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 3.00 30.02 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.02-3.00) 99.4 (30.02-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.232 , 0.288 0.229 , 0.287	Depositor DCC
R_{free} test set	1817 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 87.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10345	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.28	0/5272	0.47	0/7161
1	B	0.27	0/5176	0.47	0/7031
All	All	0.27	0/10448	0.47	0/14192

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5143	0	5096	272	0
1	B	5049	0	5005	285	0
2	B	6	0	8	0	0
3	A	74	0	0	5	0
3	B	73	0	0	2	0
All	All	10345	0	10109	553	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 27.

All (553) 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:724:ASN:HD21	1:B:730:TYR:HB3	1.10	1.15
1:A:533:THR:HB	1:A:612:THR:HG22	1.23	1.08
1:A:74:LEU:HB3	1:A:79:TYR:HE1	1.20	1.07
1:A:635:ARG:HH11	1:A:635:ARG:HG2	1.16	1.07
1:B:198:SER:HB2	1:B:202:LYS:HD3	1.48	0.96
1:A:47:ARG:HD3	1:A:47:ARG:H	1.32	0.94
1:A:422:THR:HG22	1:A:467:TRP:HE1	1.30	0.93
1:B:383:GLN:H	1:B:383:GLN:HE21	1.02	0.93
1:A:449:VAL:HG21	1:A:481:LEU:HD11	1.53	0.91
1:A:608:LYS:HG3	1:A:609:PRO:HD2	1.51	0.89
1:A:635:ARG:HG2	1:A:635:ARG:NH1	1.84	0.86
1:B:383:GLN:HE21	1:B:383:GLN:N	1.73	0.86
1:A:630:GLU:HA	1:A:689:ILE:O	1.78	0.84
1:A:691:LEU:HD21	1:A:693:ILE:HD11	1.59	0.83
1:B:94:TRP:CH2	1:B:96:PRO:HB3	2.15	0.82
1:A:74:LEU:HB3	1:A:79:TYR:CE1	2.11	0.82
1:B:536:VAL:HG22	1:B:642:PHE:HB3	1.61	0.81
1:A:532:TYR:HB3	1:A:648:LEU:HD12	1.62	0.81
1:A:179:LEU:O	1:A:183:ILE:HG12	1.79	0.81
1:B:87:GLY:HA2	1:B:107:ILE:HG23	1.62	0.80
1:B:409:VAL:HG22	1:B:445:LYS:HB3	1.64	0.80
1:B:724:ASN:ND2	1:B:730:TYR:HB3	1.95	0.79
1:A:277:ARG:HB2	1:A:280:GLU:HG3	1.66	0.78
1:A:635:ARG:HH11	1:A:635:ARG:CG	1.97	0.78
1:B:89:VAL:HG13	1:B:93:PHE:HD2	1.49	0.78
1:B:266:PHE:HB2	1:B:302:ILE:HG12	1.65	0.77
1:B:408:VAL:HG23	1:B:442:LEU:HD11	1.63	0.77
1:A:521:LEU:HD22	1:A:525:THR:HG21	1.66	0.77
1:A:312:LYS:HG2	1:A:317:ILE:HG22	1.66	0.76
1:A:529:PRO:HG2	1:A:648:LEU:HD11	1.67	0.76
1:B:697:VAL:HG13	1:B:702:VAL:HG22	1.68	0.76
1:A:86:ILE:HG13	1:A:155:ILE:HG12	1.68	0.76
1:B:89:VAL:HG13	1:B:93:PHE:CD2	2.20	0.76
1:B:537:LYS:HE2	1:B:602:PRO:HB3	1.68	0.75
1:B:529:PRO:HB3	1:B:650:LEU:HD23	1.69	0.75
1:B:312:LYS:HE3	1:B:312:LYS:N	2.02	0.74
1:B:492:GLN:HB3	1:B:522:LYS:HG3	1.69	0.74
1:B:271:GLY:O	1:B:272:LEU:HD13	1.86	0.74
1:A:315:THR:HG23	1:A:318:LYS:HE3	1.70	0.73
1:A:392:ALA:HB2	1:A:654:VAL:HG11	1.70	0.73
1:B:87:GLY:HA3	1:B:91:ARG:HD3	1.70	0.73
1:B:392:ALA:HA	1:B:654:VAL:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HG13	1:A:320:GLU:OE1	1.89	0.72
1:B:436:ARG:HH11	1:B:442:LEU:HB2	1.54	0.72
1:A:649:GLN:HA	1:A:655:MET:CB	2.19	0.72
1:B:698:ASP:HB2	1:B:703:TRP:HZ3	1.54	0.72
1:B:94:TRP:HZ2	1:B:102:ASN:HB3	1.54	0.71
1:B:508:GLU:O	1:B:509:LEU:HB2	1.89	0.71
1:A:501:LEU:HD11	1:A:648:LEU:HD22	1.71	0.71
1:B:383:GLN:H	1:B:383:GLN:NE2	1.84	0.71
1:B:405:ARG:HB2	1:B:405:ARG:HH21	1.55	0.71
1:A:48:ILE:HG21	1:A:326:ARG:HG2	1.72	0.71
1:B:155:ILE:HD13	1:B:160:LEU:HD12	1.72	0.70
1:A:206:TYR:HE2	1:A:211:ILE:HD13	1.55	0.70
1:A:89:VAL:HG13	1:A:93:PHE:CD2	2.26	0.70
1:B:532:TYR:CE1	1:B:613:PHE:HB2	2.26	0.69
1:B:70:PHE:HE2	1:B:74:LEU:HD11	1.57	0.69
1:A:406:LYS:H	1:A:406:LYS:HD2	1.58	0.69
1:B:635:ARG:HG2	1:B:635:ARG:HH11	1.58	0.69
1:B:91:ARG:HA	1:B:105:PRO:HB2	1.75	0.68
1:A:310:THR:C	1:A:312:LYS:H	1.95	0.68
1:B:449:VAL:HA	1:B:474:ILE:HG23	1.75	0.68
1:A:501:LEU:CD1	1:A:648:LEU:HD22	2.25	0.67
1:B:711:LYS:HA	1:B:716:GLU:O	1.94	0.67
1:A:196:LEU:HD11	1:A:220:TRP:HB2	1.77	0.67
1:A:646:PHE:O	1:A:658:ILE:HG22	1.95	0.67
1:B:531:LYS:HZ1	1:B:614:GLU:HB3	1.60	0.67
1:A:313:TYR:HD2	1:A:316:SER:HB3	1.59	0.67
1:A:600:TYR:O	1:A:601:ILE:HD12	1.95	0.67
1:B:86:ILE:CD1	1:B:155:ILE:HG12	2.25	0.66
1:B:411:TYR:HD2	1:B:493:PRO:HB3	1.61	0.66
1:B:700:THR:O	1:B:734:MET:HG2	1.95	0.66
1:A:419:PRO:O	1:A:423:LYS:HB2	1.97	0.65
1:B:510:SER:HB3	1:B:532:TYR:OH	1.97	0.65
1:A:555:TYR:O	1:A:558:ARG:HG2	1.96	0.65
1:B:56:THR:HA	1:B:59:VAL:HG23	1.79	0.65
1:A:422:THR:CG2	1:A:467:TRP:HE1	2.05	0.65
1:B:68:ALA:HB2	1:B:114:LEU:CD1	2.27	0.65
1:B:411:TYR:CD2	1:B:493:PRO:HB3	2.31	0.64
1:B:481:LEU:HA	1:B:484:ILE:HG12	1.79	0.64
1:A:500:LEU:O	1:A:510:SER:HB2	1.98	0.64
1:A:196:LEU:HB3	1:A:197:PRO:HD2	1.78	0.64
1:A:127:ILE:HG23	1:A:131:ILE:HD12	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD22	1:A:405:ARG:HH11	1.62	0.64
1:A:501:LEU:HD11	1:A:648:LEU:HD13	1.80	0.64
1:B:600:TYR:O	1:B:601:ILE:HD12	1.97	0.64
1:B:689:ILE:HD11	1:B:710:LYS:HG3	1.80	0.64
1:A:274:ILE:HD13	1:A:274:ILE:H	1.62	0.63
1:A:531:LYS:HB3	1:A:649:GLN:HG2	1.79	0.63
1:A:92:ALA:O	1:A:129:PRO:HD2	1.97	0.63
1:B:495:ILE:HG12	1:B:526:ILE:HG13	1.81	0.63
1:A:649:GLN:HA	1:A:655:MET:HB2	1.79	0.63
1:B:70:PHE:CE2	1:B:74:LEU:HD11	2.34	0.62
1:B:215:ASP:HB2	1:B:248:GLU:OE1	1.99	0.62
1:B:501:LEU:HD22	1:B:648:LEU:HD13	1.81	0.62
1:B:711:LYS:HE2	1:B:717:SER:HB2	1.81	0.62
1:B:593:TYR:O	1:B:673:ALA:HA	1.99	0.62
1:B:635:ARG:HG2	1:B:635:ARG:NH1	2.12	0.62
1:A:698:ASP:HB2	1:A:703:TRP:HZ3	1.64	0.62
1:B:529:PRO:HA	1:B:650:LEU:HA	1.81	0.62
1:A:53:MET:HG3	1:A:83:VAL:HB	1.81	0.62
1:A:151:GLU:O	1:A:155:ILE:HG13	2.00	0.62
1:A:86:ILE:HD11	1:A:154:TYR:HB3	1.81	0.62
1:A:400:LEU:HB3	1:A:405:ARG:HE	1.65	0.62
1:B:531:LYS:NZ	1:B:614:GLU:HB3	2.15	0.61
1:A:274:ILE:HG12	1:A:274:ILE:O	2.00	0.61
1:A:533:THR:HG23	1:A:647:ASP:OD1	2.00	0.61
1:B:724:ASN:HD21	1:B:730:TYR:CB	2.00	0.61
1:A:310:THR:HG23	1:A:310:THR:O	2.00	0.61
1:A:50:ILE:O	1:A:79:TYR:HB2	2.01	0.61
1:A:691:LEU:CD2	1:A:693:ILE:HD11	2.29	0.61
1:B:57:LEU:HD12	1:B:306:ALA:HB1	1.83	0.61
1:B:68:ALA:HB2	1:B:114:LEU:HD11	1.82	0.61
1:B:255:VAL:HG12	1:B:294:LEU:HD11	1.82	0.61
1:A:529:PRO:CG	1:A:648:LEU:HD11	2.31	0.60
1:A:292:LYS:HA	1:A:329:VAL:HG12	1.84	0.60
1:B:714:ASN:OD1	1:B:714:ASN:N	2.35	0.60
1:B:677:LEU:HD23	1:B:723:GLN:OE1	2.02	0.60
1:A:47:ARG:H	1:A:47:ARG:CD	2.11	0.60
1:B:395:GLY:HA2	1:B:398:LYS:HD3	1.83	0.60
1:A:527:SER:HB3	1:A:616:PRO:HD3	1.84	0.59
1:A:206:TYR:CE2	1:A:211:ILE:HD13	2.37	0.59
1:A:406:LYS:HD2	1:A:407:THR:H	1.67	0.59
1:A:128:SER:HB3	1:A:130:TRP:NE1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLN:CD	1:A:383:GLN:H	2.06	0.59
1:A:391:GLU:O	1:A:394:VAL:HG22	2.03	0.59
1:B:195:GLN:HG3	1:B:267:VAL:HG21	1.85	0.59
1:A:169:ARG:HD3	3:A:806:HOH:O	2.01	0.59
1:B:86:ILE:HG21	1:B:155:ILE:CD1	2.32	0.59
1:B:383:GLN:N	1:B:383:GLN:NE2	2.48	0.59
1:B:481:LEU:HD23	1:B:481:LEU:O	2.03	0.59
1:A:633:MET:HG2	1:A:683:VAL:HG21	1.85	0.58
1:A:180:LYS:HB2	1:A:227:CYS:HA	1.85	0.58
1:A:642:PHE:CD2	1:A:691:LEU:HD22	2.37	0.58
1:B:314:ASN:HB3	1:B:317:ILE:HG13	1.84	0.58
1:B:171:SER:C	1:B:173:PRO:HD3	2.24	0.58
1:A:600:TYR:H	1:A:600:TYR:HD2	1.52	0.58
1:B:69:THR:O	1:B:73:ARG:HG3	2.02	0.58
1:B:690:SER:HB2	1:B:709:GLU:HB2	1.84	0.58
1:B:196:LEU:HB3	1:B:197:PRO:HD2	1.85	0.58
1:A:407:THR:HA	1:A:443:LYS:O	2.04	0.58
1:B:182:TRP:O	1:B:186:ARG:HG2	2.04	0.58
1:B:189:ARG:HD3	1:B:234:TYR:CE1	2.39	0.58
1:B:418:GLY:N	1:B:419:PRO:HD3	2.19	0.58
1:A:562:SER:HB2	3:A:751:HOH:O	2.04	0.57
1:B:698:ASP:HB2	1:B:703:TRP:CZ3	2.36	0.57
1:A:248:GLU:HA	1:A:254:LEU:HD12	1.86	0.57
1:B:236:GLN:HB3	1:B:264:ALA:HB2	1.87	0.57
1:B:443:LYS:HE3	1:B:470:ARG:NH2	2.20	0.57
1:B:521:LEU:HD22	1:B:525:THR:HG21	1.86	0.57
1:A:591:GLN:HB2	1:A:593:TYR:CE1	2.39	0.57
1:B:326:ARG:C	1:B:328:ALA:H	2.08	0.57
1:B:668:VAL:HG12	1:B:668:VAL:O	2.05	0.57
1:A:207:ASP:C	1:A:209:PHE:H	2.08	0.57
1:B:492:GLN:HB2	1:B:522:LYS:HE2	1.86	0.57
1:A:410:ILE:HG21	1:A:424:ILE:HD13	1.87	0.56
1:B:474:ILE:HD11	1:B:484:ILE:HD12	1.87	0.56
1:A:538:PRO:HD3	1:A:631:PHE:CE1	2.41	0.56
1:B:172:SER:N	1:B:173:PRO:HD3	2.20	0.56
1:B:541:SER:HB2	1:B:600:TYR:HB2	1.87	0.56
1:A:592:ILE:HD12	1:A:675:ILE:HG13	1.88	0.55
1:B:562:SER:HB2	3:B:778:HOH:O	2.06	0.55
1:A:191:THR:HG22	1:A:192:VAL:N	2.22	0.55
1:B:646:PHE:CE2	1:B:658:ILE:HB	2.40	0.55
1:A:254:LEU:HA	1:A:257:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ILE:HD11	1:B:497:VAL:HG12	1.89	0.55
1:A:254:LEU:O	1:A:257:ARG:HD3	2.06	0.55
1:A:517:VAL:O	1:A:517:VAL:HG13	2.05	0.55
1:A:63:LEU:HD11	1:A:70:PHE:CD1	2.42	0.55
1:A:544:ILE:HB	1:A:640:MET:HE2	1.89	0.55
1:B:381:GLN:OE1	1:B:381:GLN:HA	2.07	0.55
1:B:425:LEU:HD12	1:B:467:TRP:CD1	2.41	0.55
1:B:692:LYS:HB2	1:B:707:HIS:CD2	2.41	0.55
1:B:245:LEU:HD13	1:B:287:HIS:CD2	2.42	0.55
1:B:284:PRO:HG2	1:B:287:HIS:CG	2.42	0.55
1:A:51:GLY:HA3	1:A:81:PHE:CE1	2.42	0.54
1:A:127:ILE:CG2	1:A:131:ILE:HD12	2.37	0.54
1:B:63:LEU:HD11	1:B:70:PHE:CD1	2.42	0.54
1:A:497:VAL:HG22	1:A:528:ILE:CG2	2.37	0.54
1:A:520:PHE:CG	1:A:520:PHE:O	2.60	0.54
1:A:511:PRO:O	1:A:515:ASP:HB2	2.07	0.54
1:A:648:LEU:O	1:A:655:MET:HB2	2.07	0.54
1:A:649:GLN:HA	1:A:655:MET:HB3	1.88	0.54
1:B:181:LYS:HD2	1:B:576:TRP:CZ2	2.42	0.54
1:A:255:VAL:HG12	1:A:294:LEU:HD11	1.89	0.54
1:A:582:GLN:NE2	1:A:587:ASN:HB2	2.23	0.54
1:B:312:LYS:HE3	1:B:312:LYS:H	1.72	0.54
1:B:518:THR:HA	1:B:521:LEU:HD12	1.88	0.54
1:A:451:LYS:HG3	1:A:452:ASN:N	2.21	0.54
1:B:52:TRP:O	1:B:82:VAL:HG23	2.08	0.54
1:B:450:GLU:O	1:B:475:GLU:HA	2.06	0.54
1:B:537:LYS:HB2	1:B:607:THR:HG22	1.90	0.54
1:A:70:PHE:O	1:A:74:LEU:HG	2.08	0.54
1:B:86:ILE:HD11	1:B:151:GLU:HG2	1.89	0.54
1:B:193:TRP:CH2	1:B:301:ARG:HD3	2.43	0.54
1:B:193:TRP:HH2	1:B:301:ARG:HD3	1.73	0.54
1:A:51:GLY:HA3	1:A:81:PHE:CZ	2.43	0.53
1:A:586:ARG:HD2	1:A:678:ARG:NH2	2.23	0.53
1:B:433:ASN:OD1	1:B:433:ASN:N	2.41	0.53
1:A:260:ALA:HB1	1:B:541:SER:HA	1.89	0.53
1:A:410:ILE:HD12	1:A:444:VAL:HG11	1.90	0.53
1:A:532:TYR:HB3	1:A:648:LEU:CD1	2.36	0.53
1:B:635:ARG:HH11	1:B:635:ARG:CG	2.19	0.53
1:A:257:ARG:HH21	1:B:636:ASN:HB2	1.74	0.53
1:A:659:GLU:HG2	1:A:660:PRO:HD2	1.89	0.53
1:B:423:LYS:HE3	1:B:426:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:SER:HB3	1:A:511:PRO:HD3	1.89	0.53
1:B:86:ILE:HG21	1:B:155:ILE:HD11	1.90	0.53
1:A:411:TYR:CD2	1:A:493:PRO:HB3	2.44	0.53
1:B:44:ALA:N	1:B:47:ARG:HD3	2.24	0.53
1:B:86:ILE:HD12	1:B:155:ILE:HG12	1.91	0.53
1:B:410:ILE:HG13	1:B:495:ILE:HB	1.90	0.53
1:A:308:THR:OG1	1:A:310:THR:HG22	2.09	0.53
1:A:312:LYS:HG2	1:A:317:ILE:CG2	2.36	0.53
1:A:515:ASP:O	1:A:518:THR:HG23	2.09	0.53
1:B:611:PHE:CE2	1:B:695:ARG:HB2	2.43	0.53
1:A:81:PHE:HB2	1:A:122:TYR:O	2.09	0.53
1:B:642:PHE:CD2	1:B:691:LEU:HD22	2.44	0.53
1:B:94:TRP:CZ3	1:B:96:PRO:HB3	2.43	0.53
1:B:541:SER:HB2	1:B:600:TYR:CB	2.38	0.53
1:B:86:ILE:HD13	1:B:155:ILE:HG12	1.91	0.53
1:A:77:PHE:CZ	1:A:315:THR:HG22	2.44	0.52
1:A:720:THR:HB	1:A:721:PRO:HD2	1.91	0.52
1:A:47:ARG:HD3	1:A:47:ARG:N	2.13	0.52
1:A:184:TRP:O	1:A:559:ALA:HB3	2.09	0.52
1:B:406:LYS:HD2	1:B:407:THR:HG22	1.90	0.52
1:A:537:LYS:HD3	1:A:607:THR:HG22	1.91	0.52
1:B:390:GLY:O	1:B:394:VAL:HG13	2.10	0.52
1:B:51:GLY:HA2	1:B:81:PHE:O	2.10	0.52
1:B:445:LYS:HE2	1:B:447:TYR:CE2	2.43	0.52
1:A:86:ILE:HG22	1:A:126:LYS:O	2.09	0.52
1:B:446:LEU:O	1:B:471:VAL:HG23	2.10	0.52
1:A:501:LEU:HD11	1:A:648:LEU:CD2	2.39	0.52
1:B:569:GLU:CD	1:B:579:LYS:HE2	2.29	0.52
1:A:111:ASP:HB3	1:A:158:LEU:HD23	1.92	0.52
1:A:167:LEU:HD13	3:A:755:HOH:O	2.10	0.52
1:A:310:THR:C	1:A:312:LYS:N	2.62	0.52
1:B:220:TRP:CD2	1:B:237:VAL:HB	2.45	0.52
1:A:85:PRO:HB2	1:A:92:ALA:HB2	1.92	0.51
1:A:284:PRO:O	1:A:288:ILE:HG12	2.10	0.51
1:B:273:PHE:CD2	1:B:282:SER:HB2	2.46	0.51
1:B:391:GLU:O	1:B:394:VAL:HG22	2.10	0.51
1:A:327:HIS:HA	1:A:330:ARG:HG2	1.91	0.51
1:A:70:PHE:CE2	1:A:74:LEU:HD11	2.45	0.51
1:A:645:TYR:HB3	1:A:658:ILE:HG23	1.93	0.51
1:B:77:PHE:CE2	1:B:318:LYS:HD3	2.45	0.51
1:B:86:ILE:HD11	1:B:151:GLU:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:O	1:A:76:GLU:HB2	2.10	0.51
1:A:563:HIS:HD2	1:A:591:GLN:OE1	1.93	0.51
1:A:709:GLU:HG2	1:A:719:SER:HB3	1.93	0.51
1:A:533:THR:O	1:A:646:PHE:HA	2.11	0.51
1:A:628:SER:O	1:A:629:ILE:HD13	2.11	0.51
1:B:208:ALA:HA	1:B:211:ILE:HG12	1.93	0.51
1:A:535:TYR:CD1	1:A:609:PRO:HA	2.47	0.50
1:B:77:PHE:CD2	1:B:318:LYS:HD3	2.46	0.50
1:A:274:ILE:HD13	1:A:274:ILE:N	2.26	0.50
1:A:51:GLY:HA2	1:A:81:PHE:O	2.11	0.50
1:B:423:LYS:HE3	1:B:426:LYS:CE	2.42	0.50
1:B:495:ILE:HD13	1:B:526:ILE:HD11	1.92	0.50
1:B:649:GLN:HA	1:B:655:MET:HB2	1.92	0.50
1:A:642:PHE:CZ	1:A:691:LEU:HB2	2.46	0.50
1:B:74:LEU:HB3	1:B:79:TYR:HE1	1.77	0.50
1:B:152:LEU:HB3	1:B:182:TRP:CE2	2.47	0.50
1:A:319:SER:O	1:A:322:SER:HB2	2.11	0.50
1:A:463:ASN:HA	1:A:467:TRP:HB2	1.93	0.50
1:A:724:ASN:OD1	1:A:727:GLY:HA2	2.11	0.50
1:B:405:ARG:H	1:B:405:ARG:HD3	1.76	0.50
1:B:615:HIS:HA	1:B:616:PRO:C	2.31	0.50
1:A:533:THR:HB	1:A:612:THR:CG2	2.17	0.49
1:A:249:LEU:HD13	1:A:290:LEU:HD11	1.94	0.49
1:B:422:THR:O	1:B:426:LYS:HB3	2.11	0.49
1:A:583:GLY:HA3	3:A:760:HOH:O	2.12	0.49
1:B:77:PHE:CE2	1:B:315:THR:HG22	2.47	0.49
1:B:272:LEU:HD21	1:B:287:HIS:CE1	2.47	0.49
1:A:459:LEU:HB3	1:A:473:ILE:HD12	1.94	0.49
1:B:649:GLN:HG3	1:B:649:GLN:O	2.12	0.49
1:B:240:THR:HA	1:B:267:VAL:HB	1.94	0.49
1:B:544:ILE:HB	1:B:640:MET:HE2	1.94	0.49
1:B:55:THR:HG22	1:B:57:LEU:H	1.77	0.49
1:B:387:ASP:HA	1:B:423:LYS:NZ	2.28	0.49
1:B:492:GLN:CB	1:B:522:LYS:HG3	2.42	0.49
1:B:695:ARG:HG3	1:B:704:TYR:HE2	1.77	0.49
1:A:422:THR:HG22	1:A:467:TRP:NE1	2.12	0.49
1:A:57:LEU:HD12	1:A:306:ALA:HB1	1.95	0.49
1:B:615:HIS:HA	1:B:617:ASN:N	2.28	0.49
1:A:657:SER:HB3	1:A:662:THR:O	2.13	0.48
1:A:127:ILE:HD12	1:A:127:ILE:N	2.28	0.48
1:B:56:THR:HA	1:B:59:VAL:CG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLY:C	1:B:272:LEU:HD22	2.33	0.48
1:A:207:ASP:OD2	1:A:209:PHE:HB3	2.13	0.48
1:A:317:ILE:HG13	1:A:320:GLU:CD	2.34	0.48
1:A:184:TRP:CE2	1:A:230:PHE:HD1	2.32	0.48
1:B:201:GLU:HA	1:B:206:TYR:CE2	2.48	0.48
1:B:249:LEU:O	1:B:290:LEU:HD13	2.14	0.48
1:A:527:SER:HB3	1:A:616:PRO:CD	2.44	0.48
1:B:210:THR:O	1:B:210:THR:HG22	2.14	0.48
1:B:481:LEU:N	1:B:482:PRO:CD	2.77	0.48
1:A:220:TRP:CE2	1:A:237:VAL:HB	2.49	0.48
1:A:308:THR:C	1:A:310:THR:H	2.17	0.48
1:A:541:SER:HB2	1:A:600:TYR:HA	1.96	0.48
1:A:590:ASP:HB2	1:A:729:SER:HB2	1.96	0.48
1:B:496:ILE:HG13	1:B:496:ILE:O	2.14	0.48
1:A:451:LYS:HG3	1:A:452:ASN:H	1.79	0.48
1:B:389:TYR:O	1:B:393:VAL:HG23	2.13	0.48
1:B:675:ILE:HD12	1:B:675:ILE:N	2.29	0.48
1:B:420:ILE:HD11	1:B:497:VAL:CG1	2.44	0.47
1:B:689:ILE:CD1	1:B:710:LYS:HG3	2.42	0.47
1:A:608:LYS:CG	1:A:609:PRO:HD2	2.34	0.47
1:B:703:TRP:CD1	1:B:727:GLY:N	2.82	0.47
1:A:86:ILE:C	1:A:86:ILE:HD13	2.35	0.47
1:A:312:LYS:CG	1:A:317:ILE:HG22	2.39	0.47
1:B:647:ASP:HA	1:B:657:SER:HB2	1.95	0.47
1:A:173:PRO:O	1:A:176:ALA:HB3	2.15	0.47
1:A:297:THR:O	1:A:300:LEU:HD13	2.14	0.47
1:A:646:PHE:H	1:A:658:ILE:HG22	1.80	0.47
1:B:155:ILE:HD12	1:B:163:MET:HB2	1.96	0.47
1:B:407:THR:HA	1:B:443:LYS:O	2.14	0.47
1:B:659:GLU:CD	1:B:660:PRO:HD2	2.35	0.47
1:A:593:TYR:O	1:A:673:ALA:HA	2.14	0.47
1:A:89:VAL:HG13	1:A:93:PHE:HD2	1.77	0.47
1:A:601:ILE:HD11	1:B:259:LYS:HE3	1.97	0.47
1:B:50:ILE:O	1:B:79:TYR:HB2	2.15	0.47
1:B:220:TRP:CE2	1:B:237:VAL:HB	2.49	0.47
1:B:707:HIS:CD2	1:B:707:HIS:C	2.88	0.47
1:A:165:ILE:HG23	1:A:165:ILE:O	2.14	0.47
1:B:227:CYS:HB2	3:B:783:HOH:O	2.15	0.47
1:A:220:TRP:CD2	1:A:237:VAL:HB	2.50	0.47
1:A:269:GLU:HB3	1:A:307:THR:HG21	1.97	0.47
1:A:388:VAL:HG12	1:A:650:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HG23	1:B:458:THR:HG23	1.96	0.46
1:A:51:GLY:O	1:A:303:VAL:HA	2.15	0.46
1:A:289:ASN:O	1:A:293:HIS:HB2	2.15	0.46
1:A:313:TYR:CD2	1:A:316:SER:HB3	2.44	0.46
1:B:94:TRP:CZ2	1:B:102:ASN:HB3	2.42	0.46
1:B:236:GLN:CB	1:B:264:ALA:HB2	2.44	0.46
1:B:407:THR:N	1:B:442:LEU:HD12	2.30	0.46
1:B:412:LEU:CD2	1:B:420:ILE:HG23	2.46	0.46
1:B:465:ARG:HB3	1:B:465:ARG:CZ	2.44	0.46
1:B:616:PRO:O	1:B:618:PHE:N	2.48	0.46
1:A:639:LEU:HD12	1:A:641:GLY:H	1.79	0.46
1:B:165:ILE:HG23	1:B:165:ILE:O	2.16	0.46
1:B:449:VAL:HG21	1:B:481:LEU:CD1	2.46	0.46
1:B:659:GLU:O	1:B:663:HIS:HB2	2.16	0.46
1:B:529:PRO:CA	1:B:650:LEU:HA	2.44	0.46
1:A:493:PRO:HG2	1:A:521:LEU:HD23	1.97	0.46
1:B:74:LEU:HB3	1:B:79:TYR:CE1	2.50	0.46
1:B:463:ASN:HA	1:B:467:TRP:HB2	1.96	0.46
1:A:172:SER:N	1:A:173:PRO:HD3	2.31	0.46
1:A:614:GLU:O	1:A:614:GLU:HG2	2.16	0.46
1:A:317:ILE:HA	1:A:320:GLU:CD	2.36	0.45
1:A:649:GLN:O	1:A:649:GLN:HG3	2.16	0.45
1:B:94:TRP:HB2	1:B:105:PRO:HG2	1.97	0.45
1:B:220:TRP:CE3	1:B:237:VAL:HB	2.51	0.45
1:B:506:ASP:HB2	1:B:695:ARG:HH21	1.81	0.45
1:A:695:ARG:HG3	1:A:704:TYR:HE2	1.82	0.45
1:B:195:GLN:HA	1:B:238:ALA:HB3	1.98	0.45
1:A:507:ASN:O	1:A:732:MET:SD	2.74	0.45
1:B:648:LEU:HD23	1:B:656:LEU:O	2.17	0.45
1:A:126:LYS:HB2	1:A:164:ALA:HB3	1.98	0.45
1:B:629:ILE:O	1:B:690:SER:HA	2.16	0.45
1:B:63:LEU:HD11	1:B:70:PHE:HD1	1.80	0.45
1:B:254:LEU:O	1:B:257:ARG:HB2	2.15	0.45
1:B:720:THR:HB	1:B:721:PRO:HD2	1.97	0.45
1:A:171:SER:C	1:A:173:PRO:HD3	2.37	0.45
1:A:572:GLU:H	1:A:572:GLU:CD	2.20	0.45
1:B:585:VAL:O	1:B:589:MET:HG2	2.17	0.45
1:A:401:GLY:HA3	1:A:431:TYR:OH	2.16	0.45
1:A:569:GLU:O	1:A:576:TRP:HA	2.16	0.45
1:B:477:ASP:C	1:B:479:ARG:H	2.20	0.45
1:A:75:GLY:HA2	1:A:79:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASP:HB3	1:A:158:LEU:CD2	2.47	0.45
1:A:695:ARG:HG3	1:A:704:TYR:CE2	2.52	0.45
1:A:245:LEU:HD13	1:A:287:HIS:CD2	2.53	0.45
1:A:312:LYS:HB3	1:A:317:ILE:HG22	1.98	0.45
1:A:675:ILE:N	1:A:675:ILE:HD12	2.32	0.44
1:B:85:PRO:HB2	1:B:92:ALA:HB2	1.98	0.44
1:B:486:LYS:HA	1:B:486:LYS:HD3	1.52	0.44
1:A:249:LEU:O	1:A:290:LEU:HD12	2.16	0.44
1:A:313:TYR:HD2	1:A:316:SER:CB	2.28	0.44
1:A:539:ILE:HD11	1:A:640:MET:HE1	2.00	0.44
1:B:688:ARG:NH1	1:B:711:LYS:HD2	2.32	0.44
1:A:63:LEU:HD11	1:A:70:PHE:CG	2.52	0.44
1:A:529:PRO:HA	1:A:650:LEU:HA	1.99	0.44
1:A:640:MET:SD	1:A:640:MET:C	2.95	0.44
1:B:134:ASP:OD1	1:B:173:PRO:HD2	2.18	0.44
1:B:647:ASP:CB	1:B:657:SER:HB2	2.48	0.44
1:A:530:GLN:HG3	1:A:650:LEU:O	2.18	0.44
1:B:468:LYS:HE3	1:B:468:LYS:H	1.83	0.44
1:B:478:MET:O	1:B:517:VAL:HG23	2.18	0.44
1:A:190:PHE:N	1:A:190:PHE:CD2	2.86	0.44
1:A:470:ARG:HD2	1:A:470:ARG:HA	1.69	0.44
1:A:497:VAL:HA	1:A:528:ILE:HG23	1.98	0.44
1:A:191:THR:CG2	1:A:192:VAL:N	2.81	0.44
1:A:283:ILE:CG2	1:A:287:HIS:HB3	2.48	0.44
1:A:155:ILE:HD12	1:A:163:MET:HG3	2.00	0.43
1:B:55:THR:HG22	1:B:56:THR:N	2.33	0.43
1:B:387:ASP:HA	1:B:423:LYS:HZ2	1.83	0.43
1:B:456:ILE:HG13	1:B:475:GLU:CG	2.47	0.43
1:B:689:ILE:HD13	1:B:710:LYS:HA	2.00	0.43
1:A:390:GLY:O	1:A:394:VAL:HG13	2.17	0.43
1:A:493:PRO:HG2	1:A:521:LEU:CD2	2.48	0.43
1:B:251:GLU:O	1:B:255:VAL:HG23	2.18	0.43
1:B:390:GLY:HA3	1:B:423:LYS:HE2	1.99	0.43
1:B:560:ILE:H	1:B:560:ILE:HG12	1.61	0.43
1:A:48:ILE:HG22	1:A:326:ARG:HE	1.83	0.43
1:A:295:TRP:CH2	1:A:300:LEU:O	2.71	0.43
1:A:454:ASN:O	1:A:457:VAL:HB	2.17	0.43
1:A:492:GLN:HA	1:A:520:PHE:CZ	2.54	0.43
1:A:501:LEU:HD11	1:A:648:LEU:CD1	2.46	0.43
1:B:53:MET:HB2	1:B:303:VAL:CG1	2.49	0.43
1:B:387:ASP:O	1:B:391:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:HIS:ND1	1:B:664:THR:N	2.66	0.43
1:A:109:LEU:HD11	1:A:119:TRP:HH2	1.84	0.43
1:A:423:LYS:HD2	1:A:423:LYS:HA	1.82	0.43
1:A:452:ASN:HA	1:A:453:PRO:HD3	1.80	0.43
1:A:498:SER:O	1:A:529:PRO:HD3	2.17	0.43
1:A:539:ILE:HD11	1:A:640:MET:CE	2.48	0.43
1:B:456:ILE:HG13	1:B:475:GLU:HG3	2.00	0.43
1:A:312:LYS:HD3	1:A:318:LYS:HG2	2.01	0.43
1:A:647:ASP:HB2	1:A:657:SER:HB2	1.99	0.43
1:B:174:ARG:O	1:B:178:ILE:HG12	2.19	0.43
1:B:288:ILE:HG23	1:B:292:LYS:HE3	2.01	0.43
1:B:388:VAL:HA	1:B:391:GLU:HG2	1.99	0.43
1:A:495:ILE:HA	1:A:526:ILE:O	2.18	0.43
1:B:400:LEU:HD22	1:B:405:ARG:NH1	2.34	0.43
1:B:529:PRO:HG3	1:B:648:LEU:HD12	2.01	0.43
1:A:278:ASN:OD1	1:A:280:GLU:HG2	2.19	0.43
1:A:313:TYR:CG	1:A:313:TYR:O	2.72	0.43
1:A:406:LYS:H	1:A:406:LYS:CD	2.29	0.43
1:A:668:VAL:HG12	1:A:668:VAL:O	2.19	0.43
1:B:70:PHE:O	1:B:74:LEU:HG	2.18	0.43
1:B:607:THR:CG2	1:B:660:PRO:HG2	2.49	0.43
1:A:67:VAL:HG21	1:A:109:LEU:HD11	2.01	0.43
1:A:171:SER:OG	1:A:173:PRO:HD3	2.19	0.43
1:B:126:LYS:HZ3	1:B:166:GLU:HB2	1.84	0.43
1:B:656:LEU:HD12	1:B:657:SER:N	2.34	0.43
1:A:180:LYS:O	1:A:184:TRP:HD1	2.02	0.42
1:A:724:ASN:N	1:A:725:PRO:CD	2.82	0.42
1:B:207:ASP:C	1:B:209:PHE:H	2.21	0.42
1:B:317:ILE:HA	1:B:320:GLU:HB2	2.00	0.42
1:B:692:LYS:O	1:B:706:TRP:HA	2.19	0.42
1:B:59:VAL:HG22	1:B:89:VAL:HG11	2.00	0.42
1:B:126:LYS:NZ	1:B:166:GLU:HB2	2.34	0.42
1:B:400:LEU:HD22	1:B:405:ARG:HH12	1.84	0.42
1:A:319:SER:HA	1:A:322:SER:OG	2.19	0.42
1:A:698:ASP:HA	3:A:780:HOH:O	2.18	0.42
1:B:424:ILE:HG21	1:B:446:LEU:HD13	2.02	0.42
1:A:190:PHE:N	1:A:190:PHE:HD2	2.16	0.42
1:A:385:LYS:HE2	1:A:385:LYS:HB3	1.80	0.42
1:B:418:GLY:N	1:B:419:PRO:CD	2.80	0.42
1:B:425:LEU:HA	1:B:428:GLU:HG2	2.00	0.42
1:B:557:SER:O	1:B:560:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:THR:OG1	1:A:312:LYS:HA	2.20	0.42
1:A:431:TYR:CE2	1:A:442:LEU:HD23	2.54	0.42
1:A:481:LEU:N	1:A:482:PRO:HD2	2.34	0.42
1:A:630:GLU:HG2	1:A:690:SER:HA	2.00	0.42
1:A:682:ARG:HH21	1:B:221:ALA:HB1	1.83	0.42
1:B:326:ARG:C	1:B:328:ALA:N	2.72	0.42
1:B:422:THR:HA	1:B:467:TRP:HE1	1.83	0.42
1:B:495:ILE:HG12	1:B:526:ILE:CG1	2.48	0.42
1:A:501:LEU:HD13	1:A:646:PHE:HE1	1.85	0.42
1:B:383:GLN:HG2	1:B:384:ILE:N	2.34	0.42
1:B:510:SER:N	1:B:511:PRO:CD	2.83	0.42
1:A:84:TYR:CG	1:A:85:PRO:HD2	2.55	0.42
1:A:498:SER:CB	1:A:514:LEU:HD21	2.50	0.42
1:B:500:LEU:HD13	1:B:513:CYS:SG	2.59	0.42
1:A:272:LEU:HD11	1:A:284:PRO:CD	2.50	0.42
1:A:633:MET:CE	1:A:689:ILE:HG12	2.49	0.42
1:B:68:ALA:HB2	1:B:114:LEU:HD13	1.98	0.42
1:A:253:LYS:HE2	1:A:253:LYS:HB3	1.81	0.42
1:A:539:ILE:HD13	1:A:643:ALA:HB2	2.02	0.42
1:B:116:ASN:O	1:B:120:GLU:HB2	2.20	0.42
1:B:154:TYR:CE2	1:B:158:LEU:HG	2.55	0.42
1:B:263:LEU:HD12	1:B:264:ALA:N	2.34	0.42
1:B:273:PHE:CD1	1:B:273:PHE:N	2.88	0.42
1:A:263:LEU:HD21	1:A:266:PHE:CZ	2.55	0.42
1:A:269:GLU:C	1:A:271:GLY:H	2.24	0.42
1:B:492:GLN:HA	1:B:493:PRO:HD3	1.85	0.42
1:A:694:ASP:OD1	1:A:694:ASP:N	2.53	0.41
1:B:406:LYS:HD2	1:B:406:LYS:H	1.85	0.41
1:B:428:GLU:HG3	1:B:429:ARG:N	2.35	0.41
1:B:639:LEU:HD11	1:B:641:GLY:O	2.19	0.41
1:B:240:THR:HG23	1:B:267:VAL:HB	2.02	0.41
1:B:544:ILE:HB	1:B:640:MET:CE	2.50	0.41
1:A:48:ILE:HD12	1:A:298:ASP:OD1	2.20	0.41
1:A:690:SER:HB3	1:A:692:LYS:HZ3	1.85	0.41
1:B:501:LEU:HD21	1:B:532:TYR:CD2	2.55	0.41
1:B:520:PHE:CD2	1:B:520:PHE:C	2.93	0.41
1:B:648:LEU:CD2	1:B:656:LEU:HG	2.50	0.41
1:B:411:TYR:HB2	1:B:496:ILE:HG22	2.02	0.41
1:B:423:LYS:HA	1:B:423:LYS:HD2	1.84	0.41
1:B:448:ILE:HG13	1:B:471:VAL:HG21	2.02	0.41
1:B:594:VAL:HA	1:B:672:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG12	1:A:90:VAL:O	2.20	0.41
1:A:193:TRP:HH2	1:A:301:ARG:HD3	1.85	0.41
1:A:725:PRO:O	1:A:726:ASN:CB	2.68	0.41
1:B:187:ASN:HB3	1:B:560:ILE:HG21	2.02	0.41
1:B:572:GLU:HG2	1:B:573:ASP:OD1	2.20	0.41
1:A:70:PHE:CZ	1:A:74:LEU:HD11	2.56	0.41
1:A:616:PRO:HB2	1:A:618:PHE:CE2	2.56	0.41
1:A:701:GLY:HA3	1:A:731:TYR:CZ	2.54	0.41
1:B:201:GLU:H	1:B:201:GLU:HG2	1.63	0.41
1:B:283:ILE:HG23	1:B:287:HIS:HB3	2.02	0.41
1:B:412:LEU:HD21	1:B:415:GLY:HA2	2.02	0.41
1:B:687:ASP:OD2	1:B:712:LYS:HG2	2.19	0.41
1:B:695:ARG:HG3	1:B:704:TYR:CE2	2.56	0.41
1:A:261:GLU:HA	1:A:262:PRO:HD3	1.91	0.41
1:A:389:TYR:O	1:A:393:VAL:HG23	2.21	0.41
1:A:529:PRO:CB	1:A:648:LEU:HD11	2.50	0.41
1:A:689:ILE:HD13	1:A:710:LYS:HA	2.02	0.41
1:B:189:ARG:HH22	1:B:556:LEU:HB3	1.86	0.41
1:B:382:ASP:CG	1:B:669:SER:HB2	2.41	0.41
1:B:596:TYR:C	1:B:596:TYR:CD2	2.94	0.41
1:A:302:ILE:O	1:A:302:ILE:HG22	2.21	0.41
1:A:481:LEU:N	1:A:482:PRO:CD	2.84	0.41
1:A:595:VAL:O	1:A:672:PRO:HD2	2.20	0.41
1:A:727:GLY:O	1:A:731:TYR:HB2	2.21	0.41
1:B:269:GLU:HA	1:B:305:ARG:HB3	2.03	0.41
1:B:537:LYS:CE	1:B:602:PRO:HB3	2.45	0.41
1:B:697:VAL:HG12	1:B:698:ASP:N	2.36	0.41
1:A:245:LEU:CD1	1:A:287:HIS:CD2	3.04	0.41
1:A:253:LYS:HG2	1:A:253:LYS:O	2.21	0.41
1:B:405:ARG:HD3	1:B:405:ARG:N	2.35	0.41
1:A:245:LEU:HD13	1:A:287:HIS:NE2	2.35	0.40
1:B:500:LEU:H	1:B:501:LEU:HD12	1.86	0.40
1:A:125:GLY:O	1:A:163:MET:HG2	2.21	0.40
1:A:181:LYS:HD2	1:A:576:TRP:CZ2	2.56	0.40
1:A:509:LEU:HD21	1:A:702:VAL:HB	2.02	0.40
1:A:528:ILE:CD1	1:A:650:LEU:HB3	2.51	0.40
1:A:649:GLN:HE21	1:A:649:GLN:HB2	1.65	0.40
1:B:128:SER:HB2	1:B:131:ILE:HG13	2.02	0.40
1:B:228:GLY:O	1:B:229:ASN:HB2	2.22	0.40
1:A:101:GLU:O	1:A:101:GLU:HG3	2.22	0.40
1:A:464:VAL:HG12	1:A:465:ARG:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LYS:O	1:B:184:TRP:HD1	2.03	0.40
1:B:493:PRO:HG3	1:B:520:PHE:CZ	2.57	0.40
1:B:510:SER:HB3	1:B:511:PRO:HD3	2.03	0.40
1:B:532:TYR:HB3	1:B:648:LEU:HB2	2.02	0.40
1:B:558:ARG:O	1:B:577:ILE:HD12	2.22	0.40
1:B:607:THR:HG23	1:B:660:PRO:HG2	2.02	0.40
1:B:624:GLU:O	1:B:625:ARG:HD3	2.22	0.40
1:B:700:THR:C	1:B:734:MET:HG2	2.40	0.40
1:A:295:TRP:CD2	1:A:329:VAL:HG21	2.57	0.40
1:A:297:THR:H	1:A:300:LEU:HD13	1.87	0.40
1:A:313:TYR:HB3	1:A:316:SER:HB3	2.03	0.40
1:B:52:TRP:HB2	1:B:79:TYR:CE1	2.57	0.40
1:B:390:GLY:HA3	1:B:423:LYS:NZ	2.36	0.40
1:B:410:ILE:N	1:B:410:ILE:HD12	2.37	0.40
1:B:461:TYR:CZ	1:B:465:ARG:HG3	2.56	0.40
1:B:527:SER:O	1:B:530:GLN:HG3	2.21	0.40
1:B:689:ILE:HD13	1:B:689:ILE:HA	1.88	0.40
1:A:110:PRO:HD2	1:A:113:GLN:NE2	2.36	0.40
1:B:405:ARG:O	1:B:436:ARG:NH1	2.54	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	636/745 (85%)	551 (87%)	77 (12%)	8 (1%)	12	45
1	B	620/745 (83%)	538 (87%)	77 (12%)	5 (1%)	19	57
All	All	1256/1490 (84%)	1089 (87%)	154 (12%)	13 (1%)	15	53

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	617	ASN
1	A	182	TRP
1	A	284	PRO
1	B	212	GLU
1	B	509	LEU
1	A	212	GLU
1	B	251	GLU
1	A	208	ALA
1	A	726	ASN
1	B	208	ALA
1	A	253	LYS
1	A	309	ASP
1	A	211	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	567/662 (86%)	511 (90%)	56 (10%)	8 30
1	B	557/662 (84%)	493 (88%)	64 (12%)	5 24
All	All	1124/1324 (85%)	1004 (89%)	120 (11%)	6 26

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	47	ARG
1	A	55	THR
1	A	79	TYR
1	A	80	ASN
1	A	86	ILE
1	A	161	GLN
1	A	188	SER
1	A	190	PHE
1	A	200	ILE
1	A	201	GLU

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Mol	Chain	Res	Type
1	A	213	HIS
1	A	218	THR
1	A	249	LEU
1	A	255	VAL
1	A	272	LEU
1	A	274	ILE
1	A	298	ASP
1	A	304	LEU
1	A	311	PHE
1	A	312	LYS
1	A	319	SER
1	A	327	HIS
1	A	383	GLN
1	A	406	LYS
1	A	428	GLU
1	A	462	MET
1	A	471	VAL
1	A	481	LEU
1	A	484	ILE
1	A	499	GLU
1	A	506	ASP
1	A	509	LEU
1	A	517	VAL
1	A	533	THR
1	A	536	VAL
1	A	573	ASP
1	A	575	MET
1	A	586	ARG
1	A	600	TYR
1	A	601	ILE
1	A	607	THR
1	A	614	GLU
1	A	619	MET
1	A	635	ARG
1	A	638	ASP
1	A	640	MET
1	A	648	LEU
1	A	649	GLN
1	A	653	THR
1	A	656	LEU
1	A	693	ILE
1	A	694	ASP

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Mol	Chain	Res	Type
1	A	713	THR
1	A	714	ASN
1	A	717	SER
1	B	45	ASN
1	B	56	THR
1	B	61	GLU
1	B	80	ASN
1	B	95	THR
1	B	114	LEU
1	B	117	ASP
1	B	143	LEU
1	B	151	GLU
1	B	156	CYS
1	B	163	MET
1	B	180	LYS
1	B	200	ILE
1	B	218	THR
1	B	257	ARG
1	B	263	LEU
1	B	273	PHE
1	B	291	LEU
1	B	297	THR
1	B	298	ASP
1	B	300	LEU
1	B	305	ARG
1	B	312	LYS
1	B	321	TYR
1	B	383	GLN
1	B	405	ARG
1	B	406	LYS
1	B	424	ILE
1	B	426	LYS
1	B	429	ARG
1	B	462	MET
1	B	468	LYS
1	B	472	THR
1	B	474	ILE
1	B	476	SER
1	B	486	LYS
1	B	509	LEU
1	B	520	PHE
1	B	536	VAL

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Mol	Chain	Res	Type
1	B	560	ILE
1	B	585	VAL
1	B	594	VAL
1	B	596	TYR
1	B	600	TYR
1	B	614	GLU
1	B	635	ARG
1	B	638	ASP
1	B	640	MET
1	B	648	LEU
1	B	649	GLN
1	B	652	LYS
1	B	654	VAL
1	B	656	LEU
1	B	658	ILE
1	B	659	GLU
1	B	663	HIS
1	B	667	MET
1	B	679	ASP
1	B	693	ILE
1	B	707	HIS
1	B	713	THR
1	B	714	ASN
1	B	732	MET
1	B	733	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	HIS
1	A	383	GLN
1	A	551	GLN
1	A	563	HIS
1	A	584	HIS
1	A	649	GLN
1	B	195	GLN
1	B	287	HIS
1	B	383	GLN
1	B	454	ASN
1	B	551	GLN
1	B	563	HIS
1	B	649	GLN

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Mol	Chain	Res	Type
1	B	707	HIS
1	B	724	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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	B	743	-	5,5,5	0.36	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	743	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	743	GOL	C1-C2-C3-O3
2	B	743	GOL	O2-C2-C3-O3
2	B	743	GOL	O1-C1-C2-C3
2	B	743	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	640/745 (85%)	-0.22	13 (2%)	65	36	14, 91, 179, 238	1 (0%)
1	B	628/745 (84%)	-0.10	19 (3%)	50	22	23, 101, 190, 251	15 (2%)
All	All	1268/1490 (85%)	-0.16	32 (2%)	57	29	14, 96, 183, 251	16 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	4.6
1	A	275	SER	4.4
1	B	429	ARG	4.1
1	B	97	ASN	3.8
1	B	308	THR	3.5
1	B	433	ASN	3.5
1	B	47	ARG	3.4
1	A	313	TYR	3.3
1	B	432	ASN	3.2
1	A	280	GLU	2.9
1	B	404	GLY	2.9
1	B	434	THR	2.8
1	A	278	ASN	2.7
1	B	403	ASP	2.7
1	B	316	SER	2.6
1	B	407	THR	2.6
1	A	440	GLU	2.6
1	A	99	SER	2.5
1	B	402	ALA	2.4
1	A	46	SER	2.2
1	B	430	GLU	2.2
1	B	45	ASN	2.2
1	B	101	GLU	2.2
1	B	406	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	2.2
1	A	273	PHE	2.1
1	A	274	ILE	2.1
1	B	442	LEU	2.1
1	B	310	THR	2.1
1	A	309	ASP	2.1
1	A	317	ILE	2.0
1	A	314	ASN	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	743	6/6	0.91	0.45	86,91,92,94	0

6.5 Other polymers (i)

There are no such residues in this entry.