Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

PDB ID	:	1GGY
Title	:	HUMAN FACTOR XIII WITH YTTERBIUM BOUND IN THE ION SITE
Authors	:	Fox, B.A.; Yee, V.C.; Pederson, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on	:	1998-07-23
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

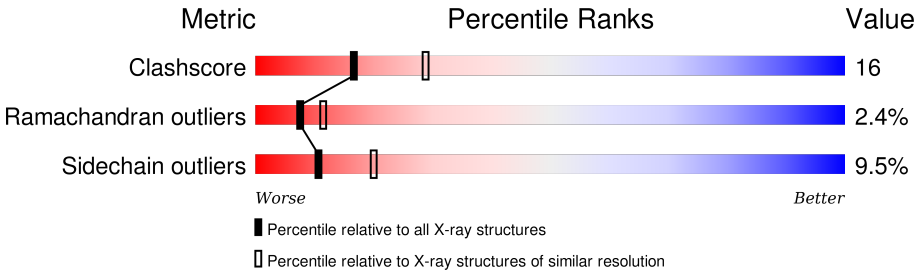
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	58% 34%
1	B	731	59% 32% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11569 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 (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	702	Total	C	N	O	S	0	0	0
			5637	3577	968	1066	26			
1	B	705	Total	C	N	O	S	0	0	0
			5659	3589	973	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	CONFLICT	UNP P00488
B	651	GLU	GLN	CONFLICT	UNP P00488

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Yb	0	0
			3	3		
2	A	5	Total	Yb	0	0
			5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total	O	0	0
			139	139		
3	B	126	Total	O	0	0
			126	126		

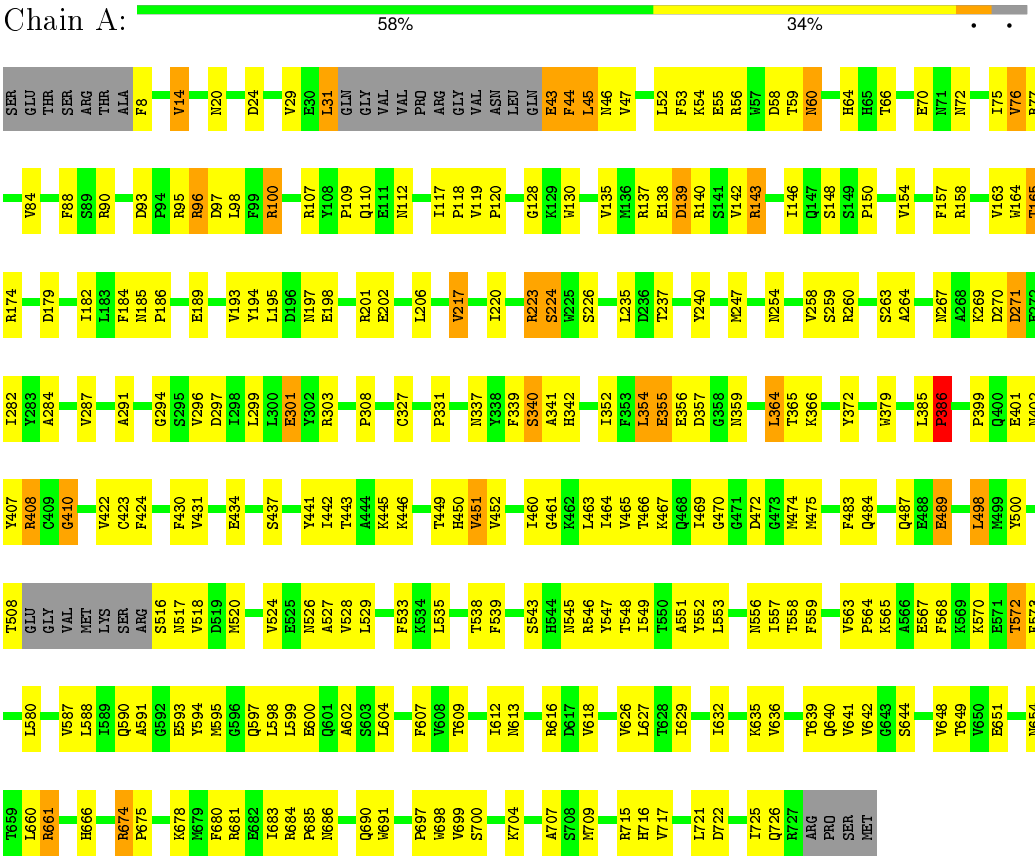
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

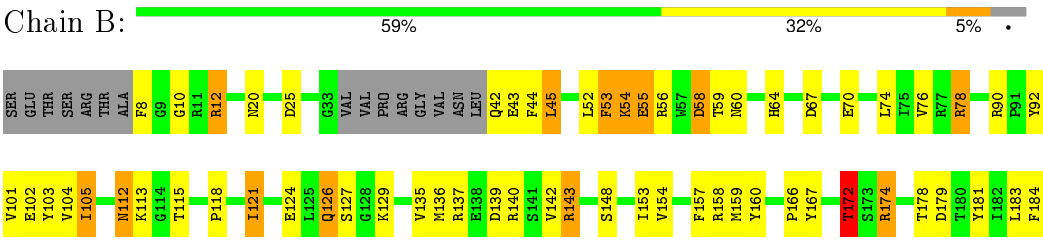
- Molecule 1: PROTEIN (COAGULATION FACTOR XIII)

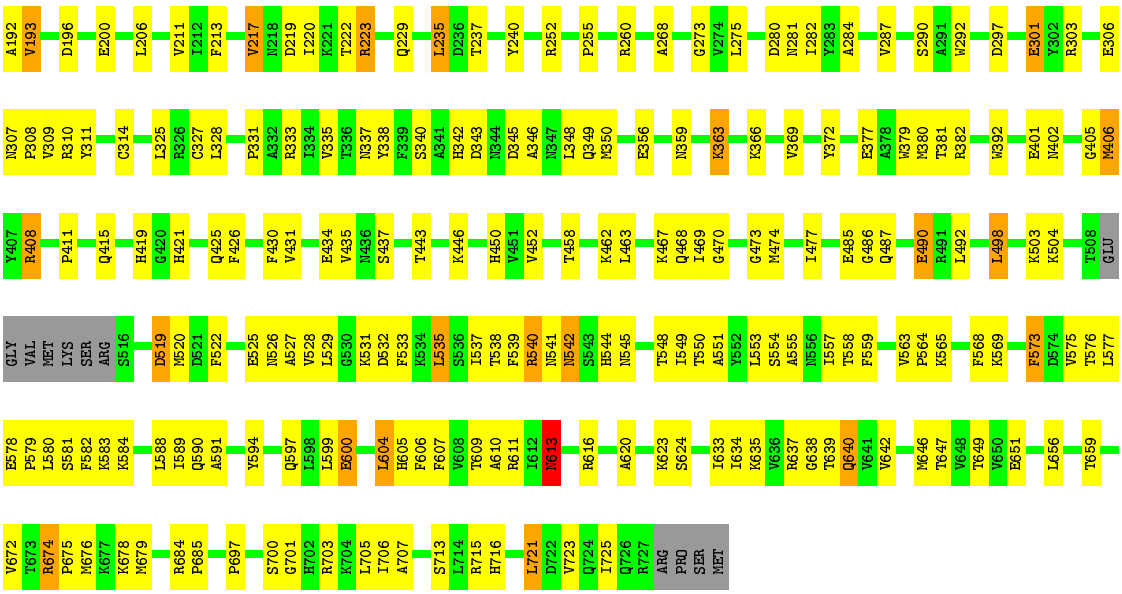
Chain A:



- Molecule 1: PROTEIN (COAGULATION FACTOR XIII)

Chain B:




A192 V193 D196 E200 L206 V211 I212 F213 V217 N218 D219 I220 K221 T222 R223 Q229 L235 D236 T237 Y240 R252 P255 R260 A268 G273 W274 L275 D280 N281 I282 Y283 A284 V287 S290 A291 W292 D297 E301 Y302 R303 E306
N307 P308 V309 R310 Y311 C314 L325 R326 C327 L328 P331 A332 R333 I334 V335 T336 N337 Y338 F339 S340 A341 H342 D343 N344 D345 A346 N347 L348 Q349 M350 E356 N359 K363 K366 V369 Y372 E377 A378 W379 M380 T381 R382 W392 E401 N402 G405 M406
Y407 R408 P411 Q415 H419 G420 H421 Q425 F426 F430 V431 E434 V435 N436 S437 T443 K446 H450 V451 V452 T458 K462 L463 K467 Q468 I469 G470 G473 M474 I477 E485 G486 Q487 E490 R491 L492 L498 K503 K504 T508 GLU
GLY VAL MET LYS SER ARG S516 D519 M520 D521 F522 E525 N526 A527 V528 L529 G530 K531 D532 F533 K534 L535 S536 I537 T538 F539 R540 N541 N542 S543 H544 N545 T548 I549 T550 A551 Y552 L553 S554 A555 N556 I557 T558 F559 V563 P564 K565 F568 K569 P573 D574 V575 T576 L577
E578 P579 L580 S581 F582 K583 K584 L588 I589 Q590 A591 V594 Q597 L598 L599 E600 L604 H605 F606 F607 V608 T609 A610 R611 I612 N613 R616 A620 K623 S624 I633 I634 K635 V636 R637 G638 T639 Q640 V641 V642 M646 T647 V648 T649 V650 E651 L656 T659
V672 T673 R674 P675 M676 K677 K678 M679 R684 P685 P697 S700 G701 H702 R703 K704 L705 I706 A707 S713 L714 R715 H716 L721 D722 V723 Q724 I725 Q726 R727 ARG PRO SER MET

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.06Å 72.39Å 135.99Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	75.9 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11569	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.56	0/5770	0.78	2/7830 (0.0%)
1	B	0.55	0/5792	0.80	2/7859 (0.0%)
All	All	0.56	0/11562	0.79	4/15689 (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	B	0	1

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	A	269	LYS	N-CA-C	-5.48	96.20	111.00
1	B	405	GLY	N-CA-C	5.20	126.09	113.10
1	A	518	VAL	N-CA-C	-5.18	97.00	111.00
1	B	604	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	TYR	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	5637	0	5489	189	0
1	B	5659	0	5508	183	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
3	A	139	0	0	7	0
3	B	126	0	0	9	0
All	All	11569	0	10997	368	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 16.

All (368) 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:220:ILE:HD13	1:B:474:MET:HE1	1.37	1.04
1:B:575:VAL:HG13	1:B:583:LYS:HD3	1.43	1.01
1:B:356:GLU:HG3	1:B:446:LYS:HD2	1.48	0.96
1:A:331:PRO:HG2	1:A:379:TRP:HB3	1.46	0.96
1:B:211:VAL:HG22	1:B:467:LYS:HD2	1.49	0.93
1:A:356:GLU:HG3	1:A:446:LYS:HG2	1.52	0.92
1:A:437:SER:HB2	1:A:460:ILE:HD12	1.55	0.87
1:B:659:THR:HG22	1:B:684:ARG:HA	1.60	0.84
1:B:44:PHE:O	1:B:45:LEU:HB2	1.78	0.83
1:A:651:GLU:HB3	1:A:690:GLN:HG3	1.60	0.81
1:B:548:THR:HB	1:B:613:ASN:HD21	1.44	0.81
1:A:95:ARG:HG2	1:A:96:ARG:HG3	1.63	0.80
1:A:8:PHE:O	1:B:563:VAL:HG11	1.85	0.77
1:A:341:ALA:HB2	1:A:460:ILE:HD13	1.64	0.76
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.68	0.75
1:A:100:ARG:HG2	1:A:164:TRP:HE1	1.50	0.75
1:A:100:ARG:HG2	1:A:164:TRP:NE1	2.01	0.75
1:B:281:ASN:OD1	1:B:600:GLU:HG3	1.88	0.73
1:A:635:LYS:HG3	1:A:649:THR:HB	1.69	0.73
1:A:64:HIS:HE1	1:A:80:GLN:HB3	1.53	0.73
1:B:345:ASP:O	1:B:503:LYS:HE2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:HIS:HA	1:B:579:PRO:HB3	1.71	0.72
1:A:443:THR:HB	1:A:451:VAL:HG13	1.70	0.72
1:A:483:PHE:HB3	1:A:487:GLN:HE21	1.55	0.72
1:A:44:PHE:HD2	1:A:90:ARG:HE	1.39	0.71
1:A:527:ALA:HB2	1:A:533:PHE:HB3	1.73	0.71
1:A:549:ILE:HB	1:A:575:VAL:HB	1.73	0.71
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.25	0.71
1:A:29:VAL:HG22	1:A:31:LEU:HD22	1.73	0.70
1:B:678:LYS:HD3	1:B:679:MET:H	1.57	0.69
1:B:537:ILE:HD12	1:B:573:PHE:HZ	1.54	0.69
1:A:467:LYS:HE2	1:A:472:ASP:HA	1.73	0.69
1:A:337:ASN:HD21	1:A:461:GLY:HA2	1.57	0.69
1:A:559:PHE:HZ	1:B:8:PHE:CD1	2.11	0.68
1:A:198:GLU:O	1:A:202:GLU:HG3	1.92	0.68
1:A:98:LEU:HD23	1:A:164:TRP:HB2	1.74	0.68
1:B:290:SER:OG	1:B:716:HIS:HD2	1.76	0.68
1:B:633:ILE:HB	1:B:651:GLU:HG3	1.76	0.68
1:B:541:ASN:HB2	1:B:577:LEU:HB3	1.75	0.67
1:A:44:PHE:O	1:A:45:LEU:HB2	1.94	0.67
1:B:126:GLN:HG3	1:B:127:SER:N	2.09	0.67
1:A:636:VAL:HG12	1:A:648:VAL:HA	1.77	0.66
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.30	0.66
1:A:90:ARG:HG3	1:A:90:ARG:HH11	1.60	0.66
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.77	0.66
1:B:172:THR:HB	3:B:3044:HOH:O	1.95	0.66
1:B:642:VAL:HG21	1:B:700:SER:HB3	1.77	0.66
1:A:557:ILE:HG21	1:A:597:GLN:O	1.96	0.66
1:B:565:LYS:HE2	1:B:597:GLN:HB2	1.79	0.65
1:A:235:LEU:HA	1:A:327:CYS:SG	2.37	0.65
1:A:157:PHE:CD1	1:A:182:ILE:HD12	2.31	0.65
1:B:78:ARG:HG2	1:B:183:LEU:O	1.97	0.65
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.33	0.64
1:B:522:PHE:O	1:B:623:LYS:HE3	1.98	0.63
1:B:280:ASP:OD2	1:B:282:ILE:HB	1.99	0.63
1:B:638:GLY:HA3	1:B:646:MET:HA	1.81	0.63
1:A:465:VAL:HG13	1:A:474:MET:HG3	1.79	0.63
1:A:237:THR:HG22	1:A:303:ARG:HD2	1.81	0.62
1:A:524:VAL:HG22	1:A:535:LEU:HG	1.80	0.62
1:B:528:VAL:HB	1:B:531:LYS:HG2	1.79	0.62
1:A:465:VAL:CG1	1:A:474:MET:HG3	2.30	0.62
1:B:557:ILE:HG21	1:B:597:GLN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:O	1:B:54:LYS:HG3	2.00	0.62
1:A:263:SER:OG	1:A:408:ARG:HD3	1.98	0.62
1:A:135:VAL:HG12	1:A:143:ARG:O	1.99	0.62
1:B:127:SER:O	1:B:129:LYS:HG3	2.01	0.61
1:A:356:GLU:HB2	1:A:446:LYS:HE2	1.83	0.61
1:B:678:LYS:HD3	1:B:679:MET:N	2.16	0.60
1:B:535:LEU:HD11	1:B:606:PHE:CD1	2.37	0.60
1:A:139:ASP:O	1:A:140:ARG:HG2	2.02	0.59
1:A:280:ASP:O	1:A:282:ILE:N	2.36	0.59
1:B:136:MET:HB3	1:B:143:ARG:HB3	1.84	0.59
1:B:105:ILE:HD11	1:B:157:PHE:CE2	2.38	0.59
1:A:254:ASN:O	1:A:258:VAL:HG23	2.03	0.58
1:B:335:VAL:HG13	1:B:477:ILE:HD11	1.85	0.57
1:B:468:GLN:HG2	1:B:473:GLY:O	2.04	0.57
1:A:547:TYR:HB3	1:A:612:ILE:HG23	1.87	0.57
1:B:193:VAL:HG13	1:B:193:VAL:O	2.04	0.57
1:B:349:GLN:HE21	1:B:504:LYS:HG3	1.69	0.57
1:B:558:THR:HG22	1:B:564:PRO:HA	1.86	0.57
1:A:90:ARG:HG3	1:A:90:ARG:NH1	2.18	0.57
1:B:656:LEU:HA	3:B:6075:HOH:O	2.04	0.56
1:A:112:ASN:HB2	3:A:3003:HOH:O	2.05	0.56
1:A:237:THR:HG22	1:A:303:ARG:CD	2.35	0.56
1:B:611:ARG:HD2	1:B:616:ARG:NH1	2.20	0.56
1:A:422:VAL:HG23	1:A:500:TYR:HB2	1.87	0.56
1:A:24:ASP:O	1:A:158:ARG:NH2	2.38	0.56
1:B:684:ARG:HB3	1:B:685:PRO:HD2	1.87	0.55
1:A:117:ILE:HG21	1:A:130:TRP:CD2	2.41	0.55
1:B:105:ILE:CD1	1:B:115:THR:HA	2.35	0.55
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.41	0.55
1:B:356:GLU:HB2	1:B:446:LYS:NZ	2.21	0.55
1:B:52:LEU:HD21	1:B:159:MET:SD	2.46	0.55
1:B:575:VAL:HG12	1:B:577:LEU:HD12	1.89	0.55
1:B:401:GLU:HA	1:B:406:MET:H	1.72	0.55
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	0.54
1:B:549:ILE:HG22	1:B:550:THR:N	2.23	0.54
1:B:273:GLY:O	1:B:308:PRO:HG3	2.07	0.54
1:B:90:ARG:HH11	1:B:90:ARG:HG3	1.71	0.54
1:A:163:VAL:HB	1:A:170:LEU:HB2	1.89	0.54
1:A:539:PHE:HB3	1:A:577:LEU:HD11	1.90	0.54
1:B:297:ASP:O	1:B:301:GLU:HB2	2.07	0.54
1:B:105:ILE:HD12	1:B:115:THR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:HA	1:A:308:PRO:HG2	1.89	0.54
1:B:634:ILE:HG22	1:B:721:LEU:HD12	1.90	0.53
1:B:485:GLU:HA	1:B:490:GLU:HG2	1.90	0.53
1:A:565:LYS:HB2	1:A:599:LEU:HD11	1.90	0.53
1:B:126:GLN:HG3	1:B:127:SER:H	1.71	0.53
1:A:70:GLU:HB3	3:A:6058:HOH:O	2.07	0.53
1:B:143:ARG:HB2	1:B:143:ARG:NH1	2.23	0.53
1:B:634:ILE:HD11	1:B:707:ALA:HB2	1.90	0.53
1:B:52:LEU:HD11	1:B:178:THR:HA	1.90	0.53
1:B:136:MET:HG2	1:B:137:ARG:N	2.24	0.53
1:B:223:ARG:NH2	3:B:6078:HOH:O	2.42	0.53
1:B:555:ALA:HB3	1:B:569:LYS:HB3	1.90	0.53
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.45	0.52
1:A:385:LEU:HD22	1:A:424:PHE:HB3	1.91	0.52
1:B:535:LEU:HD12	1:B:589:ILE:HD11	1.92	0.52
1:B:52:LEU:O	1:B:54:LYS:N	2.42	0.52
1:B:458:THR:O	1:B:462:LYS:HE3	2.09	0.52
1:A:354:LEU:HD23	1:A:618:VAL:HG11	1.92	0.52
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.40	0.52
1:B:217:VAL:HG22	1:B:338:TYR:HB3	1.92	0.51
1:A:14:VAL:HG21	1:A:110:GLN:NE2	2.26	0.51
1:A:551:ALA:HB3	1:A:573:PHE:HB2	1.92	0.51
1:B:575:VAL:CG1	1:B:583:LYS:HD3	2.30	0.51
1:A:629:ILE:HG21	1:A:717:VAL:HG22	1.92	0.51
1:A:117:ILE:HG21	1:A:130:TRP:CE2	2.46	0.51
1:A:158:ARG:HG2	1:A:174:ARG:NH2	2.26	0.51
1:A:704:LYS:HE2	1:A:722:ASP:OD1	2.11	0.51
1:B:220:ILE:HG21	1:B:474:MET:CE	2.41	0.50
1:B:540:ARG:HA	1:B:582:PHE:HA	1.93	0.50
1:B:103:TYR:HA	1:B:158:ARG:O	2.11	0.50
1:B:101:VAL:O	1:B:118:PRO:O	2.30	0.50
1:B:554:SER:HB3	1:B:607:PHE:HB2	1.92	0.50
1:A:632:ILE:HD11	1:A:709:MET:HB2	1.92	0.50
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.41	0.50
1:B:715:ARG:HG2	1:B:716:HIS:N	2.25	0.50
1:A:224:SER:HB2	3:A:3058:HOH:O	2.11	0.50
1:B:402:ASN:HA	1:B:430:PHE:CE2	2.46	0.50
1:A:53:PHE:O	1:A:60:ASN:HB2	2.12	0.50
1:B:211:VAL:HG23	1:B:467:LYS:HB2	1.93	0.50
1:B:255:PRO:HD2	3:B:3022:HOH:O	2.12	0.50
1:A:247:MET:HA	3:B:3004:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:PHE:O	1:B:60:ASN:HB2	2.11	0.50
1:B:260:ARG:NH1	1:B:408:ARG:CZ	2.74	0.50
1:B:211:VAL:CG2	1:B:467:LYS:HB2	2.42	0.49
1:A:165:THR:HB	1:A:166:PRO:HD2	1.93	0.49
1:B:609:THR:HG22	1:B:620:ALA:CB	2.41	0.49
1:A:237:THR:O	1:A:240:TYR:HB3	2.12	0.49
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.47	0.49
1:B:640:GLN:O	1:B:725:ILE:HA	2.12	0.49
1:B:672:VAL:HG11	1:B:705:LEU:HD21	1.92	0.49
1:B:443:THR:O	1:B:450:HIS:HA	2.12	0.49
1:A:260:ARG:HH11	1:A:410:GLY:HA3	1.78	0.49
1:B:260:ARG:HH12	1:B:408:ARG:CZ	2.24	0.49
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.44	0.49
1:B:54:LYS:O	1:B:55:GLU:O	2.30	0.49
1:A:364:LEU:O	1:A:366:LYS:HG2	2.13	0.49
1:B:200:GLU:HG2	1:B:469:ILE:HD11	1.93	0.49
1:A:684:ARG:H	1:A:684:ARG:HD2	1.77	0.49
1:B:90:ARG:NH1	1:B:90:ARG:HG3	2.28	0.49
1:A:641:VAL:HG12	1:A:642:VAL:O	2.13	0.49
1:A:700:SER:HA	1:A:725:ILE:HB	1.93	0.49
1:A:548:THR:HB	1:A:613:ASN:HB2	1.94	0.49
1:B:211:VAL:HG22	1:B:467:LYS:CD	2.34	0.49
1:A:437:SER:HB2	1:A:460:ILE:CD1	2.36	0.49
1:A:164:TRP:N	1:A:164:TRP:CD1	2.81	0.49
1:A:629:ILE:CG2	1:A:717:VAL:HG22	2.43	0.48
1:B:545:ASN:C	1:B:579:PRO:HG3	2.33	0.48
1:B:541:ASN:HB3	1:B:578:GLU:O	2.14	0.48
1:A:632:ILE:HG13	1:A:717:VAL:HG12	1.95	0.48
1:A:654:ASN:HB2	1:A:683:ILE:CG2	2.43	0.48
1:B:185:ASN:ND2	1:B:188:CYS:HB2	2.28	0.48
1:A:66:THR:HG21	1:A:75:ILE:HG22	1.96	0.48
1:A:517:ASN:HA	3:A:5040:HOH:O	2.13	0.48
1:B:705:LEU:O	1:B:706:ILE:HG13	2.14	0.48
1:A:93:ASP:O	1:A:97:ASP:HB2	2.14	0.48
1:A:339:PHE:O	1:A:460:ILE:HG23	2.14	0.47
1:A:220:ILE:HG21	1:A:474:MET:CE	2.44	0.47
1:A:186:PRO:HA	1:A:194:TYR:HA	1.96	0.47
1:B:539:PHE:N	1:B:539:PHE:CD1	2.82	0.47
1:B:153:ILE:HG23	1:B:252:ARG:HB2	1.96	0.47
1:A:498:LEU:HA	1:A:498:LEU:HD13	1.75	0.47
1:A:100:ARG:HB2	1:A:119:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASP:O	1:B:346:ALA:HB3	2.14	0.47
1:B:402:ASN:HA	1:B:430:PHE:CZ	2.50	0.47
1:B:356:GLU:HB2	1:B:446:LYS:HZ2	1.78	0.47
1:B:192:ALA:O	1:B:381:THR:HG23	2.13	0.47
1:A:516:SER:O	1:A:517:ASN:HB2	2.15	0.47
1:A:81:SER:HA	1:A:146:ILE:O	2.15	0.47
1:A:549:ILE:HG13	1:A:612:ILE:HD13	1.96	0.47
1:A:128:GLY:HA2	1:A:150:PRO:HD2	1.97	0.47
1:A:642:VAL:HA	1:A:697:PRO:O	2.14	0.47
1:A:567:GLU:OE2	1:A:570:LYS:HD3	2.14	0.47
1:A:117:ILE:N	1:A:117:ILE:HD12	2.29	0.47
1:A:549:ILE:HG13	1:A:612:ILE:CD1	2.45	0.47
1:B:55:GLU:HB2	1:B:58:ASP:HB2	1.97	0.47
1:B:342:HIS:O	1:B:343:ASP:HB2	2.15	0.47
1:A:197:ASN:O	1:A:201:ARG:HG3	2.15	0.47
1:A:598:LEU:HD11	1:A:627:LEU:HD12	1.96	0.47
1:B:64:HIS:CG	1:B:76:VAL:HG22	2.50	0.47
1:B:124:GLU:HB2	3:B:5056:HOH:O	2.14	0.47
1:B:349:GLN:NE2	1:B:504:LYS:HG3	2.30	0.46
1:A:52:LEU:HD23	1:A:84:VAL:HG12	1.97	0.46
1:B:56:ARG:NH1	1:B:67:ASP:O	2.43	0.46
1:B:102:GLU:HB2	1:B:160:TYR:HB2	1.97	0.46
1:B:533:PHE:CE2	1:B:589:ILE:HG13	2.50	0.46
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.45	0.46
1:B:535:LEU:HD11	1:B:606:PHE:CE1	2.50	0.46
1:A:385:LEU:HB3	1:A:386:PRO:HD2	1.96	0.46
1:B:158:ARG:HG2	1:B:174:ARG:NH2	2.31	0.46
1:A:654:ASN:HB2	1:A:683:ILE:HG21	1.97	0.46
1:B:348:LEU:HA	1:B:437:SER:HB2	1.97	0.46
1:B:549:ILE:HG21	1:B:610:ALA:HB1	1.96	0.46
1:B:380:MET:HG3	1:B:381:THR:O	2.14	0.46
1:B:237:THR:O	1:B:240:TYR:HB3	2.15	0.46
1:B:701:GLY:N	1:B:725:ILE:O	2.47	0.46
1:B:240:TYR:OH	1:B:306:GLU:HG2	2.15	0.46
1:A:297:ASP:O	1:A:301:GLU:HB2	2.15	0.46
1:B:703:ARG:NE	1:B:703:ARG:HA	2.30	0.46
1:A:423:CYS:HB3	1:A:500:TYR:CD1	2.51	0.46
1:A:602:ALA:HB1	1:A:627:LEU:HB2	1.97	0.46
1:A:138:GLU:O	1:A:140:ARG:N	2.49	0.46
1:B:44:PHE:CD1	1:B:44:PHE:N	2.84	0.46
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ARG:NH2	1:A:681:ARG:O	2.49	0.45
1:A:558:THR:HG22	1:A:564:PRO:HA	1.98	0.45
1:A:220:ILE:HD13	1:A:474:MET:HE1	1.98	0.45
1:B:333:ARG:HG2	1:B:392:TRP:CZ3	2.51	0.45
1:A:100:ARG:HE	1:A:100:ARG:HB3	1.63	0.45
1:A:590:GLN:HB3	1:A:593:GLU:HG3	1.98	0.45
1:A:107:ARG:HG2	1:A:107:ARG:O	2.15	0.45
1:A:29:VAL:O	1:A:29:VAL:HG13	2.16	0.45
1:A:580:LEU:N	1:A:580:LEU:HD12	2.32	0.45
1:A:43:GLU:HA	1:A:165:THR:CG2	2.47	0.45
1:B:542:ASN:O	1:B:580:LEU:HD23	2.15	0.45
1:B:419:HIS:HB2	1:B:421:HIS:HD2	1.82	0.45
1:B:623:LYS:HD3	3:B:6029:HOH:O	2.15	0.45
1:B:674:ARG:HG2	1:B:674:ARG:HH11	1.82	0.45
1:B:575:VAL:HG12	1:B:577:LEU:CD1	2.47	0.45
1:A:76:VAL:O	1:A:182:ILE:HA	2.17	0.45
1:B:54:LYS:HG2	1:B:74:LEU:HB2	1.98	0.45
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.46	0.45
1:A:352:ILE:HG21	1:A:441:TYR:CE1	2.52	0.45
1:A:483:PHE:CE2	1:A:489:GLU:HB2	2.52	0.44
1:B:174:ARG:NH2	1:B:179:ASP:OD1	2.50	0.44
1:A:337:ASN:ND2	1:A:464:ILE:HG12	2.32	0.44
1:A:573:PHE:HZ	1:A:587:VAL:CG2	2.30	0.44
1:B:532:ASP:OD2	1:B:590:GLN:HA	2.17	0.44
1:B:310:ARG:HB3	1:B:311:TYR:CD1	2.51	0.44
1:A:98:LEU:CD2	1:A:164:TRP:HB2	2.46	0.44
1:B:498:LEU:HD12	1:B:498:LEU:HA	1.84	0.44
1:B:153:ILE:HG22	1:B:154:VAL:N	2.32	0.44
1:B:635:LYS:HG3	1:B:649:THR:HB	1.99	0.44
1:A:674:ARG:HA	1:A:674:ARG:HD2	1.82	0.44
1:B:538:THR:HG22	1:B:584:LYS:HG3	2.00	0.44
1:A:602:ALA:O	1:A:626:VAL:HA	2.18	0.44
1:B:674:ARG:HG3	1:B:675:PRO:HD2	1.99	0.44
1:A:77:ARG:HB3	1:A:185:ASN:HB2	1.99	0.44
1:B:112:ASN:C	1:B:113:LYS:HG2	2.38	0.44
1:A:43:GLU:HA	1:A:165:THR:HG21	2.00	0.44
1:A:552:TYR:CD1	1:A:572:THR:HB	2.53	0.44
1:B:287:VAL:HB	1:B:292:TRP:CZ2	2.53	0.44
1:A:401:GLU:HA	1:A:406:MET:H	1.83	0.44
1:B:337:ASN:O	1:B:372:TYR:HA	2.17	0.44
1:A:154:VAL:HG21	1:A:184:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HA	1:B:327:CYS:SG	2.58	0.43
1:A:528:VAL:HG12	1:A:529:LEU:N	2.33	0.43
1:A:639:THR:OG1	1:A:644:SER:HB3	2.18	0.43
1:B:193:VAL:HG22	1:B:331:PRO:HD2	2.00	0.43
1:A:559:PHE:CD2	1:B:10:GLY:HA2	2.53	0.43
1:A:546:ARG:HA	1:A:577:LEU:O	2.18	0.43
1:A:354:LEU:HD22	1:A:441:TYR:HB3	1.99	0.43
1:A:287:VAL:CG1	1:A:291:ALA:HB3	2.49	0.43
1:B:559:PHE:CD1	1:B:599:LEU:HD13	2.54	0.43
1:A:79:GLY:HA2	1:A:148:SER:O	2.18	0.43
1:B:275:LEU:HA	1:B:309:VAL:O	2.19	0.43
1:A:44:PHE:HD2	1:A:90:ARG:NE	2.13	0.43
1:A:337:ASN:OD1	1:A:340:SER:HB2	2.18	0.43
1:A:678:LYS:HD3	1:A:680:PHE:CZ	2.53	0.43
1:A:220:ILE:HG21	1:A:474:MET:HE1	2.00	0.43
1:B:333:ARG:HG2	1:B:392:TRP:CH2	2.54	0.43
1:B:229:GLN:HB2	1:B:327:CYS:HB2	2.01	0.43
1:A:355:GLU:N	1:A:359:ASN:O	2.52	0.43
1:A:587:VAL:HG12	1:A:588:LEU:N	2.34	0.43
1:B:703:ARG:HB2	1:B:723:VAL:HG23	2.00	0.43
1:B:637:ARG:NH2	1:B:647:THR:HG21	2.33	0.43
1:A:337:ASN:ND2	1:A:461:GLY:HA2	2.30	0.43
1:B:126:GLN:HG2	1:B:129:LYS:HD3	2.01	0.43
1:A:189:GLU:HA	1:A:194:TYR:CG	2.54	0.43
1:A:466:THR:O	1:A:475:MET:N	2.52	0.43
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.91	0.43
1:A:666:HIS:O	1:A:707:ALA:HA	2.19	0.43
1:A:559:PHE:HD1	1:A:563:VAL:O	2.02	0.42
1:A:43:GLU:HA	1:A:165:THR:HB	2.01	0.42
1:B:703:ARG:HE	1:B:703:ARG:HA	1.83	0.42
1:A:107:ARG:C	1:A:109:PRO:HD3	2.39	0.42
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.74	0.42
1:A:709:MET:CE	1:A:717:VAL:HG21	2.49	0.42
1:B:166:PRO:HG2	1:B:167:TYR:CZ	2.53	0.42
1:A:559:PHE:HZ	1:B:8:PHE:CE1	2.36	0.42
1:B:143:ARG:HB2	1:B:143:ARG:HH11	1.83	0.42
1:A:342:HIS:ND1	1:A:434:GLU:OE2	2.52	0.42
1:A:684:ARG:N	1:A:684:ARG:HD2	2.35	0.42
1:A:399:PRO:HA	1:A:407:TYR:O	2.20	0.42
1:A:331:PRO:CG	1:A:379:TRP:HB3	2.34	0.42
1:A:543:SER:O	1:A:580:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:ARG:O	1:B:676:MET:HG3	2.20	0.42
1:A:193:VAL:HG13	1:A:331:PRO:HD2	2.01	0.42
1:B:45:LEU:HA	1:B:45:LEU:HD12	1.75	0.42
1:B:126:GLN:HE21	1:B:126:GLN:HA	1.84	0.42
1:B:705:LEU:C	1:B:706:ILE:HG13	2.40	0.42
1:B:310:ARG:HA	1:B:311:TYR:HA	1.87	0.42
1:A:88:PHE:HE2	1:A:142:VAL:CG2	2.32	0.42
1:A:281:ASN:ND2	1:A:715:ARG:NH1	2.67	0.42
1:A:445:LYS:HB2	1:A:449:THR:HB	2.00	0.42
1:A:449:THR:HG22	1:A:450:HIS:N	2.35	0.42
1:B:715:ARG:CG	1:B:716:HIS:N	2.82	0.42
1:A:44:PHE:O	1:A:45:LEU:CB	2.66	0.42
1:A:654:ASN:O	1:A:686:ASN:HA	2.20	0.42
1:A:424:PHE:HA	3:A:4006:HOH:O	2.20	0.42
1:B:350:MET:HE3	3:B:3025:HOH:O	2.19	0.42
1:A:64:HIS:CD2	1:A:76:VAL:HG12	2.55	0.42
1:B:401:GLU:HA	1:B:406:MET:N	2.35	0.42
1:B:158:ARG:HG2	1:B:174:ARG:CZ	2.50	0.42
1:B:363:LYS:O	1:B:366:LYS:HE2	2.20	0.41
1:A:264:ALA:HA	1:A:408:ARG:HG2	2.02	0.41
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.53	0.41
1:A:558:THR:C	1:A:599:LEU:HD12	2.41	0.41
1:A:674:ARG:HG3	1:A:675:PRO:HD2	2.03	0.41
1:A:469:ILE:HD11	3:A:3080:HOH:O	2.19	0.41
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.83	0.41
1:A:726:GLN:HA	1:A:726:GLN:HE21	1.85	0.41
1:A:193:VAL:HG13	1:A:331:PRO:CD	2.51	0.41
1:A:557:ILE:HG13	1:A:568:PHE:CD1	2.56	0.41
1:B:555:ALA:HB1	1:B:568:PHE:CZ	2.55	0.41
1:B:12:ARG:HH11	1:B:12:ARG:CB	2.32	0.41
1:A:118:PRO:O	1:A:120:PRO:HD3	2.20	0.41
1:A:337:ASN:HD22	1:A:464:ILE:HG12	1.86	0.41
1:B:605:HIS:HD2	1:B:624:SER:OG	2.03	0.41
1:B:42:GLN:OE1	1:B:44:PHE:HE1	2.04	0.41
1:B:600:GLU:OE2	1:B:715:ARG:HD2	2.21	0.41
1:B:335:VAL:HG21	1:B:377:GLU:HG3	2.03	0.41
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.56	0.41
1:A:656:LEU:HD12	1:A:660:LEU:HD21	2.03	0.41
1:A:504:LYS:HB3	1:A:504:LYS:HE2	1.96	0.41
1:B:697:PRO:CB	1:B:725:ILE:HD13	2.51	0.41
1:A:658:GLU:C	1:A:685:PRO:HG3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:NH2	3:A:5021:HOH:O	2.53	0.41
1:B:425:GLN:HA	1:B:426:PHE:HA	1.79	0.41
1:A:217:VAL:HG11	1:A:339:PHE:CE2	2.56	0.41
1:A:337:ASN:O	1:A:372:TYR:HA	2.21	0.41
1:A:226:SER:HB3	1:A:294:GLY:HA3	2.01	0.41
1:B:307:ASN:HA	1:B:308:PRO:HD3	1.93	0.40
1:A:563:VAL:HA	1:A:564:PRO:HD3	1.85	0.40
1:A:280:ASP:CG	1:A:280:ASP:O	2.60	0.40
1:A:442:ILE:HG12	1:A:452:VAL:HG12	2.03	0.40
1:B:121:ILE:H	1:B:121:ILE:HD13	1.86	0.40
1:B:519:ASP:HB2	3:B:4008:HOH:O	2.19	0.40
1:B:45:LEU:HD22	1:B:97:ASP:HB3	2.02	0.40
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.86	0.40
1:B:105:ILE:HG13	1:B:157:PHE:CD2	2.57	0.40
1:A:709:MET:HE3	1:A:717:VAL:HG21	2.03	0.40
1:B:486:GLY:O	1:B:487:GLN:HG3	2.22	0.40
1:B:184:PHE:HD2	1:B:328:LEU:O	2.05	0.40
1:B:92:TYR:HD2	1:B:137:ARG:HD3	1.85	0.40
1:B:551:ALA:HA	1:B:610:ALA:HA	2.03	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	696/731 (95%)	617 (89%)	60 (9%)	19 (3%)	6 9
1	B	699/731 (96%)	620 (89%)	65 (9%)	14 (2%)	9 15
All	All	1395/1462 (95%)	1237 (89%)	125 (9%)	33 (2%)	7 11

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	139	ASP
1	B	45	LEU
1	B	55	GLU
1	B	600	GLU
1	A	54	LYS
1	A	55	GLU
1	A	56	ARG
1	A	270	ASP
1	A	273	GLY
1	A	281	ASN
1	A	296	VAL
1	A	410	GLY
1	B	53	PHE
1	B	219	ASP
1	B	284	ALA
1	B	314	CYS
1	B	406	MET
1	A	595	MET
1	A	600	GLU
1	B	54	LYS
1	B	268	ALA
1	A	217	VAL
1	A	284	ALA
1	A	365	THR
1	A	716	HIS
1	B	581	SER
1	B	613	ASN
1	A	60	ASN
1	A	386	PRO
1	B	172	THR
1	B	470	GLY
1	A	470	GLY

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	619/644 (96%)	563 (91%)	56 (9%)	12 22
1	B	621/644 (96%)	559 (90%)	62 (10%)	9 18
All	All	1240/1288 (96%)	1122 (90%)	118 (10%)	11 20

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

Mol	Chain	Res	Type
1	A	14	VAL
1	A	20	ASN
1	A	31	LEU
1	A	43	GLU
1	A	44	PHE
1	A	46	ASN
1	A	47	VAL
1	A	58	ASP
1	A	59	THR
1	A	72	ASN
1	A	76	VAL
1	A	96	ARG
1	A	100	ARG
1	A	137	ARG
1	A	143	ARG
1	A	165	THR
1	A	195	LEU
1	A	206	LEU
1	A	223	ARG
1	A	224	SER
1	A	259	SER
1	A	267	ASN
1	A	271	ASP
1	A	281	ASN
1	A	301	GLU
1	A	340	SER
1	A	354	LEU
1	A	355	GLU
1	A	357	ASP
1	A	364	LEU
1	A	386	PRO
1	A	404	ASP
1	A	408	ARG
1	A	431	VAL
1	A	451	VAL

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Mol	Chain	Res	Type
1	A	463	LEU
1	A	484	GLN
1	A	489	GLU
1	A	498	LEU
1	A	508	THR
1	A	520	MET
1	A	526	ASN
1	A	538	THR
1	A	545	ASN
1	A	553	LEU
1	A	556	ASN
1	A	572	THR
1	A	574	ASP
1	A	604	LEU
1	A	607	PHE
1	A	609	THR
1	A	616	ARG
1	A	640	GLN
1	A	661	ARG
1	A	674	ARG
1	A	721	LEU
1	B	12	ARG
1	B	20	ASN
1	B	25	ASP
1	B	43	GLU
1	B	58	ASP
1	B	59	THR
1	B	70	GLU
1	B	78	ARG
1	B	98	LEU
1	B	104	VAL
1	B	105	ILE
1	B	112	ASN
1	B	121	ILE
1	B	126	GLN
1	B	135	VAL
1	B	139	ASP
1	B	140	ARG
1	B	142	VAL
1	B	143	ARG
1	B	148	SER
1	B	172	THR

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Mol	Chain	Res	Type
1	B	174	ARG
1	B	193	VAL
1	B	196	ASP
1	B	206	LEU
1	B	217	VAL
1	B	223	ARG
1	B	235	LEU
1	B	301	GLU
1	B	303	ARG
1	B	340	SER
1	B	359	ASN
1	B	363	LYS
1	B	369	VAL
1	B	408	ARG
1	B	415	GLN
1	B	431	VAL
1	B	435	VAL
1	B	452	VAL
1	B	463	LEU
1	B	490	GLU
1	B	492	LEU
1	B	498	LEU
1	B	519	ASP
1	B	520	MET
1	B	525	GLU
1	B	526	ASN
1	B	529	LEU
1	B	535	LEU
1	B	540	ARG
1	B	542	ASN
1	B	553	LEU
1	B	573	PHE
1	B	576	THR
1	B	588	LEU
1	B	604	LEU
1	B	613	ASN
1	B	639	THR
1	B	640	GLN
1	B	674	ARG
1	B	713	SER
1	B	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	72	ASN
1	A	337	ASN
1	A	373	HIS
1	A	556	ASN
1	A	726	GLN
1	B	72	ASN
1	B	112	ASN
1	B	126	GLN
1	B	421	HIS
1	B	545	ASN
1	B	605	HIS
1	B	613	ASN
1	B	686	ASN
1	B	716	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.