

Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 05:57 pm BST

PDB ID	:	2AYN
Title	:	Structure of USP14, a proteasome-associated deubiquitinating enzyme
Authors	:	Hu, M.; Li, P.; Jeffrey, P.D.; Shi, Y.
Deposited on	:	2005-09-07
Resolution	:	3.20 Å(reported)

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

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.20 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	Similar resolution	
	(# Entries)	(#Entries, resolution range(A))	
Clashscore	141614	1253 (3.20-3.20)	
Ramachandran outliers	138981	1234 (3.20-3.20)	
Sidechain outliers	138945	1233 (3.20-3.20)	

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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain			
1	А	404	37%	41%	5%	17%
1	В	404	36%	41%	6%	17%
1	С	404	35%	41%	7% •	17%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8163 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	227	Total	С	Ν	Ο	S	0	0	0
	A	001	2721	1734	447	521	19	0	0	0
1	р	227	Total	С	Ν	Ο	S	0	0	0
	D	001	2721	1734	447	521	19	0	0	0
1	C	227	Total	С	Ν	Ο	S	0	0	0
		337	2721	1734	447	521	19		U	U

• Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.



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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are colorcoded 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. 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: Ubiquitin carboxyl-terminal hydrolase 14







CLIN S317 THR S317 THR S317 THR S231 THR S231 ASN S231 ASN S231 ASN S231 ASN S231 ASN S231 ASN S232 ELYS S321 ELYS S323 ELYS S323 ELAS C2325 ELAS C3325 ELAS C3335 E4041 C334 A406 C344 A416 C345 A416 C345 A416 C345 A416 C345 A416 C345 A416 C345 A416

D450 D451 D451 D451 D451 D452 C457 C457 D4456 C457 D4456 C457 D4456 D4456 C447 D4464 D4475 D4476 D4477 D4478 D4488 </t

• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	82.28Å 121.58Å 166.85Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	99.00 - 3.20	Depositor	
% Data completeness	(Not available) (99.00-3.20)	Depositor	
(in resolution range)	(1101 available) (55.00 5.20)	Depositor	
R_{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	CNS	Depositor	
R, R_{free}	0.261 , 0.322	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	8163	wwPDB-VP	
Average B, all atoms $(Å^2)$	123.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond	lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/2772	0.75	0/3732
1	В	0.57	0/2772	0.76	0/3732
1	С	0.50	0/2772	0.72	0/3732
All	All	0.54	0/8316	0.75	0/11196

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 (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	А	2721	0	2696	169	0
1	В	2721	0	2696	200	0
1	С	2721	0	2696	190	0
All	All	8163	0	8088	544	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 33.

All (544) 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:C:184:GLN:N	1:C:184:GLN:HE21	1.45	1.14



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1·C·184·GLN·H	1.C.184.GLN.NE2	1 44	1 13
1:B:184:GLN:H	1:B:184:GLN:NE2	1.50	1.08
1:A:184:GLN:H	1:A:184:GLN:NE2	1.50	1.08
1:B:172:ILE:HD11	1:C:109:LEU:HB3	1.34	1.06
1:A:350:LEU:HD11	1:A:463:LEU:HD21	1.37	1.05
1:B:184:GLN:N	1:B:184:GLN:HE21	1.54	1.04
1:A:184:GLN:N	1:A:184:GLN:HE21	1.56	1.04
1:B:350:LEU:HD11	1:B:463:LEU:HD21	1.41	1.01
1:B:260:GLU:HG2	1:B:304:LEU:HD11	1.43	0.99
1:B:457:VAL:HG22	1:B:458:THR:H	1.29	0.96
1:C:260:GLU:HG2	1:C:304:LEU:HD11	1.50	0.92
1:A:260:GLU:HG2	1:A:304:LEU:HD11	1.51	0.92
1:C:350:LEU:HD11	1:C:463:LEU:HD21	1.51	0.91
1:B:109:LEU:HB3	1:C:172:ILE:HD11	1.55	0.89
1:B:300:GLN:HA	1:B:307:ASN:HA	1.55	0.88
1:A:457:VAL:HG22	1:A:458:THR:H	1.38	0.88
1:B:172:ILE:CD1	1:C:109:LEU:HB3	2.05	0.87
1:C:187:GLU:HG3	1:C:195:LEU:HD12	1.58	0.84
1:C:343:LEU:HD12	1:C:343:LEU:N	1.93	0.83
1:C:150:TYR:HB3	1:C:177:PHE:CD2	2.14	0.82
1:C:457:VAL:HG22	1:C:458:THR:H	1.45	0.81
1:A:462:ILE:H	1:A:462:ILE:HD12	1.45	0.81
1:B:462:ILE:HD12	1:B:462:ILE:H	1.46	0.81
1:C:448:LYS:HB3	1:C:455:SER:HB3	1.60	0.81
1:B:109:LEU:HB3	1:C:172:ILE:CD1	2.11	0.81
1:B:457:VAL:HG22	1:B:458:THR:N	1.96	0.80
1:C:300:GLN:HA	1:C:307:ASN:HA	1.64	0.80
1:A:424:THR:HG21	1:A:472:HIS:HB3	1.65	0.79
1:C:304:LEU:N	1:C:304:LEU:HD12	1.98	0.79
1:C:424:THR:HG21	1:C:472:HIS:HB3	1.65	0.78
1:A:460:GLU:H	1:A:460:GLU:CD	1.86	0.78
1:B:172:ILE:HD11	1:C:109:LEU:CB	2.14	0.78
1:C:115:MET:O	1:C:119:VAL:HG23	1.83	0.78
1:C:417:TYR:HB3	1:C:479:TYR:HB3	1.66	0.78
1:A:300:GLN:HA	1:A:307:ASN:HA	1.66	0.77
1:A:343:LEU:HD12	1:A:343:LEU:H	1.51	0.76
1:B:258:GLU:O	1:B:260:GLU:N	2.18	0.76
1:C:153:ALA:O	1:C:156:ARG:HG3	1.84	0.76
1:B:350:LEU:N	1:B:350:LEU:HD12	2.02	0.75
1:A:459:PRO:HA	1:A:462:ILE:HD13	1.68	0.75
1:B:277:PHE:HB2	1:B:292:ARG:NH1	2.03	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1:A:205:GLN:NE2	1:A:205:GLN:HA	2.03	0.73
1:A:350:LEU:CD1	1:A:463:LEU:HD21	2.18	0.73
1:A:191:GLN:C	1:A:193:GLN:H	1.92	0.73
1:A:153:ALA:O	1:A:156:ARG:HG3	1.88	0.73
1:C:158:LEU:O	1:C:162:MET:HG3	1.88	0.73
1:A:304:LEU:N	1:A:304:LEU:HD12	2.03	0.72
1:B:150:TYR:HB3	1:B:177:PHE:CD2	2.24	0.72
1:A:172:ILE:HD13	1:B:164:LYS:O	1.90	0.72
1:C:150:TYR:HB3	1:C:177:PHE:HD2	1.53	0.72
1:C:334:GLU:OE2	1:C:335:LYS:HG3	1.90	0.72
1:C:363:GLN:O	1:C:367:VAL:HG23	1.90	0.72
1:B:270:ASN:O	1:B:271:GLN:HG3	1.90	0.71
1:B:459:PRO:HA	1:B:462:ILE:HD13	1.72	0.71
1:C:405:PHE:CZ	1:C:481:PRO:HG3	2.26	0.71
1:C:457:VAL:HG22	1:C:461:ASP:OD2	1.90	0.71
1:A:457:VAL:HG22	1:A:461:ASP:OD2	1.91	0.71
1:A:283:LYS:HA	1:A:283:LYS:HE2	1.73	0.71
1:A:210:LEU:HD22	1:A:214:LEU:HD11	1.72	0.70
1:A:164:LYS:O	1:A:166:SER:N	2.24	0.70
1:B:241:LEU:O	1:B:244:GLN:HB2	1.90	0.70
1:C:262:GLU:OE1	1:C:302:PRO:HG2	1.92	0.70
1:B:424:THR:HG21	1:B:472:HIS:HB3	1.74	0.70
1:B:208:ARG:O	1:B:211:GLN:HB3	1.92	0.69
1:B:417:TYR:HB3	1:B:479:TYR:HB3	1.73	0.69
1:B:351:MET:CE	1:B:482:ARG:HG3	2.23	0.69
1:A:150:TYR:HB3	1:A:177:PHE:CD2	2.27	0.69
1:C:343:LEU:HD12	1:C:343:LEU:H	1.58	0.69
1:B:165:THR:HG22	1:B:167:SER:OG	1.92	0.69
1:B:164:LYS:O	1:B:166:SER:N	2.24	0.69
1:A:248:VAL:HG22	1:A:320:PRO:HD3	1.74	0.68
1:B:262:GLU:OE1	1:B:302:PRO:HD2	1.93	0.68
1:B:460:GLU:CD	1:B:460:GLU:H	1.95	0.68
1:C:277:PHE:HB2	1:C:292:ARG:NH1	2.08	0.68
1:A:407:ASP:OD1	1:A:414:CYS:HB3	1.94	0.68
1:C:448:LYS:CB	1:C:455:SER:HB3	2.23	0.68
1:A:417:TYR:HB3	1:A:479:TYR:HB3	1.75	0.68
1:B:260:GLU:HG2	1:B:304:LEU:CD1	2.21	0.68
1:C:350:LEU:HD12	1:C:350:LEU:N	2.09	0.68
1:B:256:CYS:HB2	1:B:310:TYR:CE2	2.29	0.68
1:C:460:GLU:H	1:C:460:GLU:CD	1.96	0.68
1:A:457:VAL:HG22	1:A:458:THR:N	2.10	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan(Å)
1.C.240.SEB.HB2	$1 \cdot C \cdot 243 \cdot ASP \cdot OD2$	1.94	0.67
1:C:258:GLU:O	1:C:260:GLU:N	2.28	0.67
1:A:258:GLU:O	1:A:260:GLU:N	2.20	0.67
1:A:196:GLN:HB3	1:A:431:SEB:O	1.95	0.67
1:C:198:ASP:HB3	1:C:201:GLU:HB2	1.76	0.67
1:B:253:THR:HG22	1:B:266:LYS:HD3	1.77	0.67
1:C:459:PRO:HA	1:C:462:ILE:HD13	1.75	0.67
1:B:248:VAL:HG22	1:B:320:PRO:HD3	1.76	0.66
1:B:330:PHE:CD1	1:B:341:LYS:HB2	2.30	0.66
1:C:205:GLN:O	1:C:209:VAL:HG23	1.95	0.66
1:C:210:LEU:HD22	1:C:214:LEU:HD11	1.78	0.66
1:B:150:TYR:HB3	1:B:177:PHE:CE2	2.31	0.66
1:B:211:GLN:HA	1:B:242:ILE:HG13	1.77	0.66
1:B:109:LEU:CB	1:C:172:ILE:HD11	2.24	0.66
1:B:127:GLU:HG2	1:B:245:PHE:CE2	2.31	0.66
1:B:283:LYS:HE2	1:B:283:LYS:HA	1.78	0.66
1:C:114:TYR:CD1	1:C:197:GLN:HB2	2.30	0.65
1:C:283:LYS:HA	1:C:283:LYS:HE2	1.77	0.65
1:C:462:ILE:HD12	1:C:462:ILE:H	1.61	0.65
1:B:148:ALA:HB1	1:B:209:VAL:HG13	1.78	0.65
1:C:164:LYS:O	1:C:166:SER:N	2.30	0.65
1:C:196:GLN:HB3	1:C:431:SER:O	1.97	0.64
1:C:407:ASP:OD1	1:C:414:CYS:HB3	1.96	0.64
1:B:457:VAL:HG22	1:B:461:ASP:OD2	1.96	0.64
1:B:200:ASN:O	1:B:204:ILE:HG13	1.98	0.64
1:A:424:THR:CG2	1:A:472:HIS:HB3	2.27	0.64
1:A:247:GLY:O	1:A:320:PRO:HB3	1.98	0.64
1:C:304:LEU:N	1:C:304:LEU:CD1	2.61	0.64
1:C:165:THR:HG22	1:C:167:SER:OG	1.99	0.63
1:B:205:GLN:NE2	1:B:205:GLN:HA	2.12	0.63
1:A:269:GLU:OE1	1:A:312:LYS:NZ	2.26	0.63
1:C:423:LEU:HB3	1:C:476:VAL:HB	1.80	0.63
1:A:241:LEU:O	1:A:244:GLN:HB2	2.00	0.62
1:B:304:LEU:N	1:B:304:LEU:HD12	2.13	0.62
1:C:270:ASN:O	1:C:271:GLN:HG3	1.99	0.62
1:A:343:LEU:HD12	1:A:343:LEU:N	2.14	0.62
1:A:256:CYS:HB2	1:A:310:TYR:CE2	2.35	0.62
1:A:429:SER:HB3	1:A:432:SER:HB3	1.81	0.62
1:B:342:VAL:C	1:B:343:LEU:HD12	2.21	0.61
1:A:270:ASN:O	1:A:271:GLN:HG3	2.00	0.61
1:C:352:LEU:O	1:C:416:TYR:HB3	1.99	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:405:PHE:CZ	1:A:481:PRO:HG3	2.35	0.61
1:C:256:CYS:HB2	1:C:310:TYR:CE2	2.35	0.61
1:C:446:TRP:CG	1:C:462:ILE:HD11	2.35	0.61
1:B:138:ALA:H	1:B:149:GLN:HE22	1.48	0.61
1:B:405:PHE:CZ	1:B:481:PRO:HG2	2.35	0.61
1:A:127:GLU:HG2	1:A:245:PHE:CE2	2.36	0.61
1:C:150:TYR:HB3	1:C:177:PHE:CE2	2.36	0.61
1:C:260:GLU:HG2	1:C:304:LEU:CD1	2.28	0.60
1:A:217:ILE:HG22	1:A:218:GLU:N	2.16	0.60
1:A:208:ARG:O	1:A:211:GLN:HB3	2.00	0.60
1:A:205:GLN:O	1:A:209:VAL:HG23	2.02	0.60
1:B:153:ALA:O	1:B:156:ARG:HG3	2.01	0.60
1:B:424:THR:CG2	1:B:472:HIS:HB3	2.32	0.60
1:B:240:SER:HB2	1:B:243:ASP:OD2	2.02	0.60
1:C:248:VAL:HG22	1:C:320:PRO:HD3	1.83	0.60
1:C:253:THR:HG22	1:C:266:LYS:HD3	1.84	0.60
1:A:351:MET:CE	1:A:482:ARG:HG3	2.31	0.59
1:B:126:PRO:O	1:B:128:LEU:N	2.35	0.59
1:B:249:GLU:HG2	1:B:270:ASN:OD1	2.02	0.59
1:C:260:GLU:HG3	1:C:262:GLU:HG3	1.84	0.59
1:C:341:LYS:O	1:C:343:LEU:HD11	2.03	0.59
1:B:418:ASP:N	1:B:480:GLY:O	2.25	0.59
1:C:424:THR:CG2	1:C:472:HIS:HB3	2.30	0.59
1:A:249:GLU:HG2	1:A:270:ASN:OD1	2.03	0.59
1:A:350:LEU:N	1:A:350:LEU:HD12	2.17	0.58
1:B:350:LEU:CD1	1:B:463:LEU:HD21	2.26	0.58
1:C:211:GLN:HA	1:C:242:ILE:HG13	1.85	0.58
1:A:251:GLU:HG3	1:A:317:SER:HB2	1.84	0.58
1:B:458:THR:O	1:B:461:ASP:HB2	2.02	0.58
1:B:345:ASP:HA	1:B:467:GLY:HA3	1.84	0.58
1:C:303:THR:HB	1:C:304:LEU:HD12	1.86	0.58
1:A:148:ALA:HB1	1:A:209:VAL:HG13	1.84	0.58
1:C:351:MET:CE	1:C:482:ARG:HG3	2.33	0.58
1:B:363:GLN:O	1:B:367:VAL:HG23	2.03	0.58
1:C:158:LEU:HD23	1:C:162:MET:HG3	1.86	0.58
1:B:163:ASP:O	1:B:164:LYS:HG3	2.03	0.58
1:A:338:VAL:HG21	1:C:337:SER:HB2	1.86	0.58
1:A:423:LEU:HB3	1:A:476:VAL:HB	1.86	0.58
1:B:362:LEU:HD22	1:B:366:MET:HE2	1.85	0.58
1:A:165:THR:HG22	1:A:167:SER:OG	2.03	0.57
1:A:262:GLU:OE1	1:A:302:PRO:HD2	2.04	0.57



Interatomic Clash				
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:B:118:THR:HG22	1:B:122:ILE:HD11	1.86	0.57	
1:A:150:TYR:HB3	1:A:177:PHE:HD2	1.70	0.57	
1:A:277:PHE:HB2	1:A:292:ARG:NH1	2.20	0.57	
1:A:122:ILE:O	1:A:128:LEU:HD23	2.04	0.57	
1:A:240:SER:HB2	1:A:243:ASP:OD2	2.05	0.57	
1:B:115:MET:O	1:B:119:VAL:HG23	2.04	0.57	
1:B:351:MET:HE1	1:B:482:ARG:HG3	1.87	0.57	
1:B:462:ILE:HD12	1:B:462:ILE:N	2.17	0.57	
1:C:283:LYS:NZ	1:C:344:LYS:HE2	2.20	0.57	
1:B:138:ALA:H	1:B:149:GLN:NE2	2.03	0.57	
1:C:122:ILE:O	1:C:128:LEU:HD23	2.05	0.57	
1:B:407:ASP:OD1	1:B:414:CYS:HB3	2.05	0.57	
1:B:196:GLN:HB3	1:B:431:SER:O	2.05	0.57	
1:A:260:GLU:HG2	1:A:304:LEU:CD1	2.30	0.56	
1:A:425:HIS:HB2	1:A:435:TYR:CD2	2.40	0.56	
1:C:331:PHE:H	1:C:331:PHE:HD2	1.51	0.56	
1:A:115:MET:HE3	1:A:178:LEU:HD22	1.88	0.56	
1:A:205:GLN:HE21	1:A:205:GLN:HA	1.70	0.56	
1:C:217:ILE:HG22	1:C:218:GLU:N	2.20	0.56	
1:A:114:TYR:CD1	1:A:197:GLN:HB2	2.41	0.56	
1:C:158:LEU:CD2	1:C:162:MET:HG3	2.35	0.56	
1:C:316:ILE:O	1:C:362:LEU:HD12	2.05	0.56	
1:C:425:HIS:HB2	1:C:435:TYR:CE2	2.41	0.56	
1:C:148:ALA:HB1	1:C:209:VAL:HG13	1.87	0.56	
1:B:355:TYR:O	1:B:357:LEU:N	2.39	0.55	
1:B:457:VAL:CG2	1:B:458:THR:H	2.09	0.55	
1:C:350:LEU:CD1	1:C:463:LEU:HD21	2.31	0.55	
1:A:304:LEU:N	1:A:304:LEU:CD1	2.68	0.55	
1:B:205:GLN:O	1:B:209:VAL:HG23	2.07	0.55	
1:B:217:ILE:HG22	1:B:218:GLU:N	2.22	0.55	
1:B:198:ASP:HB3	1:B:201:GLU:HB2	1.88	0.55	
1:A:360:PRO:HA	1:A:363:GLN:OE1	2.07	0.55	
1:A:211:GLN:HA	1:A:242:ILE:HG13	1.88	0.55	
1:B:147:SER:HB3	1:B:181:ALA:HB2	1.89	0.55	
1:B:448:LYS:HB3	1:B:455:SER:HB3	1.88	0.55	
1:B:277:PHE:HB2	1:B:292:ARG:HH11	1.70	0.55	
1:B:360:PRO:HA	1:B:363:GLN:OE1	2.05	0.55	
1:A:150:TYR:HB3	1:A:177:PHE:CE2	2.41	0.55	
1:B:247:GLY:O	1:B:320:PRO:HB3	2.06	0.55	
1:B:199:ALA:HB2	1:B:435:TYR:CD2	2.42	0.55	
1:B:112:THR:O	1:B:115:MET:N	2.35	0.55	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:260:GLU:HG3	1:B:262:GLU:HG3	1.88	0.54	
1:C:457:VAL:HG22	1:C:458:THR:N	2.18	0.54	
1:A:184:GLN:H	1:A:184:GLN:HE21	0.71	0.54	
1:A:345:ASP:HA	1:A:467:GLY:HA3	1.90	0.54	
1:A:106:LEU:HD22	1:A:171:PRO:HG3	1.88	0.54	
1:B:351:MET:HE2	1:B:482:ARG:HG3	1.88	0.54	
1:B:352:LEU:O	1:B:416:TYR:HB3	2.07	0.54	
1:C:355:TYR:C	1:C:357:LEU:H	2.10	0.54	
1:A:115:MET:CE	1:A:178:LEU:HD22	2.37	0.54	
1:C:355:TYR:O	1:C:357:LEU:N	2.40	0.53	
1:A:158:LEU:HD22	1:A:162:MET:SD	2.48	0.53	
1:A:198:ASP:HB3	1:A:201:GLU:HB2	1.90	0.53	
1:B:341:LYS:HG2	1:B:343:LEU:HD11	1.89	0.53	
1:C:360:PRO:HA	1:C:363:GLN:OE1	2.09	0.53	
1:A:260:GLU:OE1	1:A:262:GLU:HG2	2.08	0.53	
1:B:274:LEU:O	1:B:325:ILE:HA	2.08	0.53	
1:B:341:LYS:HG2	1:B:343:LEU:CD1	2.39	0.53	
1:A:172:ILE:HD13	1:B:164:LYS:HA	1.90	0.53	
1:A:352:LEU:O	1:A:416:TYR:HB3	2.08	0.53	
1:B:128:LEU:O	1:B:129:LYS:C	2.47	0.53	
1:C:200:ASN:O	1:C:203:TRP:HB3	2.09	0.53	
1:C:401:GLU:N	1:C:402:PRO:CD	2.72	0.53	
1:C:401:GLU:N	1:C:402:PRO:HD2	2.23	0.52	
1:A:198:ASP:C	1:A:198:ASP:OD1	2.48	0.52	
1:A:316:ILE:O	1:A:362:LEU:HD12	2.09	0.52	
1:B:462:ILE:CD1	1:B:462:ILE:H	2.20	0.52	
1:C:202:CYS:O	1:C:206:MET:HG3	2.09	0.52	
1:C:274:LEU:O	1:C:325:ILE:HA	2.10	0.52	
1:B:304:LEU:N	1:B:304:LEU:CD1	2.72	0.52	
1:B:425:HIS:HB2	1:B:435:TYR:CE2	2.45	0.52	
1:C:351:MET:HE1	1:C:482:ARG:HG3	1.89	0.52	
1:B:330:PHE:CE1	1:B:341:LYS:HD2	2.45	0.52	
1:C:200:ASN:HD21	1:C:273:GLN:NE2	2.08	0.52	
1:C:329:ARG:NH2	1:C:344:LYS:O	2.41	0.52	
1:B:423:LEU:HB3	1:B:476:VAL:HB	1.92	0.51	
1:A:329:ARG:HH21	1:A:343:LEU:HA	1.75	0.51	
1:B:172:ILE:HD11	1:C:109:LEU:HD22	1.91	0.51	
1:B:416:TYR:CD1	1:B:416:TYR:N	2.78	0.51	
1:B:425:HIS:HB2	1:B:435:TYR:CD2	2.46	0.51	
1:C:200:ASN:O	1:C:204:ILE:HG13	2.10	0.51	
1:B:429:SER:HB3	1:B:432:SER:HB3	1.92	0.51	



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlan (Å)		
1.A.115.MET.HE1	1·A·174·LEU·HG	1.93	0.51		
1:A:401:GLU:N	1:A:402:PRO:HD2	2.26	0.51		
1:A:410:GLY:O	1:A:411:SEB:CB	2.59	0.51		
1:B:362:LEU:HD22	1:B:366:MET:CE	$\frac{2.30}{2.40}$	0.51		
1:A:115:MET:O	1:A:116:ASN:C	2.47	0.51		
1:C:182:PHE:C	1:C:184:GLN:NE2	2.63	0.51		
1:C:205:GLN:NE2	1:C:205:GLN:HA	2.26	0.51		
1:A:446:TRP:CG	1:A:462:ILE:HD11	2.46	0.51		
1:A:205:GLN:HE21	1:A:205:GLN:CA	2.23	0.51		
1:B:198:ASP:O	1:B:199:ALA:C	2.48	0.50		
1:B:401:GLU:N	1:B:402:PBO:HD2	$\frac{2.19}{2.25}$	0.50		
1:A:286:PHE:O	1:A:287:THB:C	2.49	0.50		
1:A:200:ASN:HB2	1:A:475:TYB:CE2	2.46	0.50		
1:C:120:GLN:O	1:C:123:ARG:HG2	2.12	0.50		
1:B:401:GLU:N	1:B:402:PBO:CD	2 75	0.50		
1:B:449:PHE:O	1:B:451:ASP:N	2.42	0.50		
1:C:424:THR:HB	1:C:438:TRP:HE1	1 76	0.50		
1:A:200:ASN:O	1:A:204:ILE:HG13	2.12	0.50		
1:A:424:THR:HB	1:A:438:TRP:HE1	1.77	0.50		
1:C:208:ARG:O	1:C:211:GLN:HB3	2.12	0.50		
1:A:260:GLU:HG3	1:A:260:GLU:O	2.12	0.50		
1:B:211:GLN:CA	1:B:242:ILE:HG13	2.41	0.49		
1:A:363:GLN:O	1:A:367:VAL:HG23	2.11	0.49		
1:B:211:GLN:HA	1:B:242:ILE:CG1	2.41	0.49		
1:C:277:PHE:HB2	1:C:292:ARG:HH11	1.74	0.49		
1:B:350:LEU:N	1:B:350:LEU:CD1	2.74	0.49		
1:B:109:LEU:HD22	1:C:172:ILE:HD11	1.93	0.49		
1:C:331:PHE:CD2	1:C:331:PHE:N	2.78	0.49		
1:C:425:HIS:HB2	1:C:435:TYR:CD2	2.47	0.49		
1:A:211:GLN:HA	1:A:242:ILE:CG1	2.42	0.49		
1:A:200:ASN:HD21	1:A:273:GLN:NE2	2.11	0.49		
1:B:159:PHE:O	1:B:162:MET:HB2	2.12	0.49		
1:C:163:ASP:O	1:C:164:LYS:HG3	2.12	0.49		
1:A:351:MET:HE2	1:A:482:ARG:HG3	1.94	0.49		
1:A:371:SER:C	1:A:373:PHE:H	2.16	0.49		
1:B:115:MET:CE	1:B:175:LEU:HA	2.42	0.49		
1:B:366:MET:O	1:B:370:ARG:HB2	2.13	0.49		
1:C:362:LEU:HD22	1:C:366:MET:HE2	1.95	0.49		
1:A:129:LYS:O	1:A:132:LEU:HB2	2.12	0.49		
1:A:191:GLN:C	1:A:193:GLN:N	2.63	0.49		
1:B:122:ILE:O	1:B:128:LEU:HD23	2.12	0.49		



		Interatomic	Clash		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1:C:187:GLU:HG3	1:C:195:LEU:CD1	2.38	0.49		
1:C:345:ASP:HA	1:C:467:GLY:HA3	1.94	0.49		
1:B:150:TYR:HB3	1:B:177:PHE:HD2	1.73	0.49		
1:A:401:GLU:N	1:A:402:PRO:CD	2.76	0.49		
1:A:460:GLU:O	1:A:464:ARG:HG3	2.12	0.49		
1:B:126:PRO:C	1:B:128:LEU:N	2.65	0.49		
1:A:457:VAL:CG2	1:A:461:ASP:CG	2.82	0.49		
1:B:191:GLN:C	1:B:193:GLN:H	2.16	0.48		
1:B:448:LYS:CB	1:B:455:SER:HB3	2.43	0.48		
1:A:355:TYR:O	1:A:357:LEU:N	2.46	0.48		
1:A:447:ILE:HG22	1:A:448:LYS:O	2.13	0.48		
1:B:371:SER:C	1:B:373:PHE:H	2.15	0.48		
1:A:329:ARG:HH21	1:A:343:LEU:C	2.17	0.48		
1:C:304:LEU:CD1	1:C:304:LEU:H	2.27	0.48		
1:C:429:SER:HB3	1:C:432:SER:CB	2.43	0.48		
1:B:210:LEU:HD22	1:B:214:LEU:HD11	1.95	0.48		
1:C:115:MET:HE1	1:C:174:LEU:HG	1.96	0.48		
1:A:325:ILE:HG22	1:A:327:MET:HE2	1.95	0.48		
1:B:158:LEU:HD22	1:B:162:MET:SD	2.53	0.48		
1:C:158:LEU:HD22	1:C:162:MET:SD	2.54	0.48		
1:C:331:PHE:HD2	1:C:331:PHE:N	2.10	0.48		
1:C:159:PHE:O	1:C:162:MET:HB2	2.13	0.48		
1:C:442:LYS:HB3	1:C:445:GLU:HB3	1.95	0.48		
1:B:118:THR:O	1:B:122:ILE:HG13	2.13	0.48		
1:B:163:ASP:C	1:B:164:LYS:HG3	2.34	0.48		
1:B:440:LYS:HB2	1:B:446:TRP:CE2	2.49	0.48		
1:C:416:TYR:N	1:C:416:TYR:CD1	2.82	0.48		
1:B:278:ILE:HD12	1:B:329:ARG:HG2	1.95	0.48		
1:B:401:GLU:O	1:B:402:PRO:C	2.51	0.48		
1:C:114:TYR:CG	1:C:197:GLN:HB2	2.48	0.48		
1:C:125:VAL:CG1	1:C:128:LEU:HB2	2.43	0.48		
1:C:303:THR:HB	1:C:304:LEU:CD1	2.44	0.48		
1:A:448:LYS:HB3	1:A:455:SER:HB3	1.96	0.48		
1:B:248:VAL:HG22	1:B:320:PRO:CD	2.43	0.48		
1:B:257:THR:N	1:B:309:LEU:O	2.46	0.48		
1:B:139:LEU:HD23	1:B:139:LEU:O	2.14	0.47		
1:B:114:TYR:CD1	1:B:197:GLN:HB2	2.49	0.47		
1:B:252:THR:N	1:B:267:GLY:O	2.43	0.47		
1:C:217:ILE:HG22	1:C:218:GLU:H	1.79	0.47		
1:C:251:GLU:HG3	1:C:317:SER:HB2	1.95	0.47		
1:A:457:VAL:HG22	1:A:461:ASP:CG	2.35	0.47		



	Clash			
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:459:PRO:C	1:B:461:ASP:N	2.65	0.47	
1:C:158:LEU:O	1:C:158:LEU:HD23	2.13	0.47	
1:A:351:MET:HE1	1:A:482:ARG:HG3	1.94	0.47	
1:C:297:ILE:O	1:C:309:LEU:HD23	2.14	0.47	
1:C:374:LYS:C	1:C:376:LEU:H	2.17	0.47	
1:A:355:TYR:C	1:A:357:LEU:H	2.17	0.47	
1:C:106:LEU:HD22	1:C:171:PRO:HG3	1.96	0.47	
1:B:410:GLY:N	1:B:412:ASN:HD21	2.12	0.47	
1:B:248:VAL:HG12	1:B:249:GLU:N	2.30	0.47	
1:B:410:GLY:O	1:B:411:SER:CB	2.63	0.47	
1:A:172:ILE:CD1	1:B:164:LYS:HA	2.45	0.47	
1:A:401:GLU:O	1:A:402:PRO:C	2.52	0.47	
1:B:260:GLU:OE1	1:B:262:GLU:HG2	2.15	0.47	
1:B:374:LYS:C	1:B:376:LEU:H	2.18	0.47	
1:A:455:SER:OG	1:A:456:ILE:N	2.46	0.47	
1:B:204:ILE:H	1:B:204:ILE:HG13	1.50	0.47	
1:C:325:ILE:HG22	1:C:327:MET:CE	2.45	0.47	
1:C:429:SER:H	1:C:432:SER:HB3	1.80	0.47	
1:B:270:ASN:C	1:B:271:GLN:HG3	2.35	0.46	
1:B:115:MET:HE1	1:B:175:LEU:HA	1.95	0.46	
1:B:355:TYR:C	1:B:357:LEU:H	2.17	0.46	
1:B:442:LYS:HB3	1:B:445:GLU:HB3	1.97	0.46	
1:C:114:TYR:CE1	1:C:197:GLN:HB2	2.51	0.46	
1:C:118:THR:HG22	1:C:122:ILE:HD11	1.97	0.46	
1:C:401:GLU:O	1:C:402:PRO:C	2.54	0.46	
1:A:209:VAL:O	1:A:210:LEU:C	2.52	0.46	
1:A:416:TYR:CD1	1:A:416:TYR:N	2.83	0.46	
1:B:405:PHE:HB3	1:B:406:ALA:H	1.42	0.46	
1:A:277:PHE:HB2	1:A:292:ARG:HH11	1.81	0.46	
1:A:458:THR:O	1:A:461:ASP:HB2	2.16	0.46	
1:B:158:LEU:HD22	1:B:162:MET:HG3	1.98	0.46	
1:C:450:ASP:HB3	1:C:453:LYS:HB2	1.98	0.46	
1:A:362:LEU:HD22	1:A:366:MET:HE2	1.97	0.46	
1:A:460:GLU:N	1:A:460:GLU:CD	2.63	0.46	
1:A:101:GLU:O	1:A:102:LEU:HG	2.15	0.46	
1:A:200:ASN:O	1:A:203:TRP:HB3	2.16	0.46	
1:B:475:TYR:O	1:B:475:TYR:CD1	2.68	0.46	
1:A:442:LYS:HB3	1:A:445:GLU:HB3	1.98	0.46	
1:B:199:ALA:CB	1:B:435:TYR:CE2	2.99	0.46	
1:C:259:SER:O	1:C:260:GLU:C	2.54	0.46	
1:C:211:GLN:CA	1:C:242:ILE:HG13	2.46	0.46	



	Interatomic Clash				
Atom-1	Atom-2	distance $(Å)$	overlan (Å)		
1:C:241:LEU:O	1:C:244:GLN:HB2	2.15	0.45		
1:C:429:SER:HB3	1:C:432:SER:HB3	1.97	0.45		
1:C:106:LEU:O	1:C:451:ASP:C	2.55	0.45		
1:A:187:GLU:OE1	1:C:428:ARG:HG2	2.16	0.45		
1:B:242:ILE:C	1:B:244:GLN:N	2.67	0.45		
1:A:125:VAL:O	1:A:128:LEU:HB3	2.17	0.45		
1:A:374:LYS:C	1:A:376:LEU:H	2.20	0.45		
1:B:344:LYS:HD3	1:B:344:LYS:HA	1.68	0.45		
1:C:209:VAL:O	1:C:210:LEU:C	2.55	0.45		
1:A:405:PHE:HB3	1:A:406:ALA:H	1.47	0.45		
1:B:460:GLU:O	1:B:464:ARG:HG3	2.15	0.45		
1:C:424:THR:O	1:C:424:THR:HG22	2.16	0.45		
1:A:159:PHE:O	1:A:162:MET:HB2	2.16	0.45		
1:A:462:ILE:H	1:A:462:ILE:CD1	2.23	0.45		
1:C:127:GLU:HG2	1:C:245:PHE:CE2	2.52	0.45		
1:C:458:THR:O	1:C:461:ASP:HB2	2.17	0.45		
1:A:123:ARG:O	1:A:129:LYS:HE3	2.17	0.45		
1:A:158:LEU:O	1:A:162:MET:HG3	2.16	0.45		
1:A:184:GLN:N	1:A:184:GLN:NE2	2.35	0.45		
1:A:348:PHE:O	1:A:348:PHE:CD1	2.69	0.45		
1:B:424:THR:HB	1:B:438:TRP:HE1	1.81	0.45		
1:C:270:ASN:O	1:C:271:GLN:CG	2.63	0.45		
1:C:405:PHE:HB3	1:C:406:ALA:H	1.54	0.45		
1:A:425:HIS:HB2	1:A:435:TYR:CE2	2.52	0.45		
1:B:283:LYS:O	1:B:346:VAL:HA	2.16	0.45		
1:C:249:GLU:HG2	1:C:270:ASN:OD1	2.17	0.45		
1:C:118:THR:O	1:C:122:ILE:HG13	2.17	0.45		
1:A:401:GLU:O	1:A:403:PHE:N	2.50	0.45		
1:B:260:GLU:HG3	1:B:260:GLU:O	2.17	0.45		
1:B:109:LEU:HD12	1:B:175:LEU:HD22	1.99	0.44		
1:B:457:VAL:CG2	1:B:461:ASP:CG	2.86	0.44		
1:A:344:LYS:HA	1:A:344:LYS:HD3	1.79	0.44		
1:C:126:PRO:O	1:C:128:LEU:N	2.50	0.44		
1:C:199:ALA:HB2	1:C:435:TYR:CD2	2.52	0.44		
1:C:418:ASP:N	1:C:480:GLY:O	2.40	0.44		
1:B:242:ILE:C	1:B:244:GLN:H	2.21	0.44		
1:C:125:VAL:O	1:C:128:LEU:HB3	2.17	0.44		
1:C:211:GLN:HA	1:C:242:ILE:CG1	2.46	0.44		
1:A:429:SER:HB3	1:A:432:SER:CB	2.47	0.44		
1:B:135:TYR:CG	1:B:136:ALA:N	2.85	0.44		
1:B:352:LEU:HD21	1:B:354:MET:SD $ $	2.57	0.44		



		Interatomic	Clash		
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
1:A:135:TYR:CG	1:A:136:ALA:N	2.85	0.44		
1:A:260:GLU:HG3	1:A:262:GLU:HG3	2.00	0.44		
1:B:211:GLN:O	1:B:240:SER:HB3	2.17	0.44		
1:C:115:MET:HE3	1:C:178:LEU:HD22	2.00	0.44		
1:A:440:LYS:HB2	1:A:446:TRP:CE2	2.53	0.44		
1:A:449:PHE:O	1:A:451:ASP:N	2.48	0.44		
1:A:461:ASP:O	1:A:462:ILE:C	2.56	0.44		
1:C:240:SER:O	1:C:243:ASP:HB2	2.17	0.44		
1:C:423:LEU:CB	1:C:476:VAL:HB	2.45	0.44		
1:B:115:MET:HE1	1:B:174:LEU:HG	2.00	0.44		
1:C:125:VAL:HG12	1:C:128:LEU:H	1.83	0.44		
1:A:114:TYR:CG	1:A:197:GLN:HB2	2.52	0.43		
1:B:278:ILE:HG22	1:B:278:ILE:O	2.17	0.43		
1:B:292:ARG:HG2	1:B:292:ARG:NH1	2.33	0.43		
1:B:459:PRO:C	1:B:461:ASP:H	2.21	0.43		
1:C:200:ASN:HD21	1:C:273:GLN:HE22	1.65	0.43		
1:A:429:SER:H	1:A:432:SER:HB3	1.83	0.43		
1:B:125:VAL:O	1:B:128:LEU:HB3	2.18	0.43		
1:B:203:TRP:CD1	1:B:203:TRP:C	2.92	0.43		
1:B:325:ILE:HG22	1:B:327:MET:CE	2.47	0.43		
1:B:424:THR:O	1:B:424:THR:HG22	2.18	0.43		
1:B:334:GLU:C	1:B:336:GLU:H	2.21	0.43		
1:A:173:ILE:HG13	1:A:173:ILE:H	1.60	0.43		
1:A:321:ALA:HA	1:A:413:ASN:HB2	1.99	0.43		
1:B:158:LEU:CD2	1:B:162:MET:HG3	2.49	0.43		
1:B:369:PHE:O	1:B:373:PHE:CD2	2.71	0.43		
1:A:162:MET:C	1:A:164:LYS:H	2.22	0.43		
1:B:148:ALA:CB	1:B:209:VAL:HG13	2.47	0.43		
1:C:204:ILE:H	1:C:204:ILE:HG13	1.51	0.43		
1:C:446:TRP:CD2	1:C:462:ILE:HD11	2.53	0.43		
1:A:139:LEU:HD23	1:A:139:LEU:O	2.18	0.43		
1:B:184:GLN:N	1:B:184:GLN:NE2	2.34	0.43		
1:B:401:GLU:O	1:B:403:PHE:N	2.51	0.43		
1:A:164:LYS:O	1:A:165:THR:C	2.57	0.43		
1:A:248:VAL:HG22	1:A:320:PRO:CD	2.47	0.43		
1:B:184:GLN:H	1:B:184:GLN:HE21	0.69	0.43		
1:C:193:GLN:O	1:C:193:GLN:CG	2.66	0.43		
1:B:109:LEU:HB2	1:B:112:THR:HG21	2.00	0.43		
1:B:257:THR:CB	1:B:309:LEU:O	2.67	0.43		
1:B:303:THR:HB	1:B:304:LEU:HD12	2.01	0.43		
1:A:217:ILE:HG22	1:A:218:GLU:H	1.82	0.43		



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:126:PRO:O	1:B:127:GLU:C	2.57	0.43
1:C:163:ASP:C	1:C:164:LYS:HG3	2.39	0.43
1:A:172:ILE:HG21	1:B:164:LYS:O	2.18	0.43
1:A:270:ASN:C	1:A:271:GLN:HG3	2.39	0.43
1:A:276:CYS:SG	1:A:276:CYS:O	2.75	0.43
1:C:371:SER:C	1:C:373:PHE:H	2.22	0.42
1:C:457:VAL:HG22	1:C:461:ASP:CG	2.39	0.42
1:A:115:MET:O	1:A:119:VAL:HG23	2.19	0.42
1:C:148:ALA:CB	1:C:209:VAL:HG13	2.48	0.42
1:B:199:ALA:HB3	1:B:435:TYR:CE2	2.55	0.42
1:C:124:SER:O	1:C:126:PRO:HD3	2.19	0.42
1:A:163:ASP:O	1:A:164:LYS:HG3	2.19	0.42
1:C:422:VAL:O	1:C:438:TRP:HD1	2.03	0.42
1:A:362:LEU:O	1:A:365:LYS:N	2.53	0.42
1:B:329:ARG:O	1:B:342:VAL:N	2.36	0.42
1:C:199:ALA:CB	1:C:435:TYR:CD2	3.03	0.42
1:C:260:GLU:OE1	1:C:262:GLU:HG2	2.20	0.42
1:A:211:GLN:CA	1:A:242:ILE:HG13	2.48	0.42
1:A:217:ILE:CG2	1:A:218:GLU:N	2.83	0.42
1:B:106:LEU:HD22	1:B:171:PRO:HG3	2.02	0.42
1:B:300:GLN:HB2	1:B:307:ASN:OD1	2.20	0.42
1:B:198:ASP:OD1	1:B:198:ASP:C	2.58	0.42
1:C:210:LEU:HD22	1:C:214:LEU:CD1	2.48	0.42
1:C:410:GLY:O	1:C:411:SER:CB	2.67	0.42
1:C:460:GLU:O	1:C:464:ARG:HG3	2.19	0.42
1:A:193:GLN:CG	1:A:193:GLN:O	2.67	0.42
1:A:199:ALA:HB2	1:A:435:TYR:CD2	2.54	0.42
1:C:138:ALA:H	1:C:149:GLN:HE22	1.67	0.42
1:C:270:ASN:C	1:C:271:GLN:HG3	2.39	0.42
1:A:106:LEU:O	1:A:451:ASP:C	2.57	0.42
1:A:478:LEU:C	1:A:478:LEU:CD2	2.89	0.42
1:B:151:ILE:HD11	1:B:178:LEU:HA	2.00	0.42
1:B:164:LYS:O	1:B:165:THR:C	2.57	0.42
1:B:179:HIS:O	1:B:180:MET:C	2.57	0.42
1:B:270:ASN:O	1:B:271:GLN:CG	2.65	0.42
1:C:327:MET:O	1:C:329:ARG:HG3	2.19	0.42
1:A:203:TRP:CD1	1:A:203:TRP:C	2.94	0.41
1:B:165:THR:HG22	1:B:167:SER:HG	1.83	0.41
1:C:125:VAL:HG12	1:C:128:LEU:HB2	2.02	0.41
1:C:292:ARG:HD3	1:C:292:ARG:HA	1.85	0.41
1:C:306:ARG:HD2	1:C:306:ARG:O	2.20	0.41



Interatomic Clash						
Atom-1	Atom-2	distance $(Å)$	overlap (Å)			
1:B:205:GLN:NE2	1:B:205:GLN:CA	2.75	0.41			
1:B:450:ASP:HB3	1:B:453:LYS:HB2	2.02	0.41		0.41	
1:A:211:GLN:O	1:A:240:SER:HB3	2.20	0.41			
1:B:321:ALA:O	1:B:481:PRO:HD3	2.19	0.41			
1:C:446:TRP:CE2	1:C:462:ILE:HG12	2.56	0.41			
1:A:164:LYS:C	1:A:166:SER:N	2.73	0.41			
1:A:301:SER:HA	1:A:302:PRO:HD3	1.59	0.41			
1:A:355:TYR:OH	1:A:363:GLN:HB3	2.20	0.41			
1:B:330:PHE:HD1	1:B:341:LYS:HB2	1.82	0.41			
1:C:164:LYS:O	1:C:165:THR:C	2.57	0.41			
1:C:210:LEU:HB3	1:C:214:LEU:HD12	2.01	0.41			
1:B:199:ALA:CB	1:B:435:TYR:CD2	3.03	0.41			
1:B:205:GLN:HE21	1:B:205:GLN:CA	2.32	0.41			
1:A:245:PHE:HB3	1:A:322:TYR:HD1	1.86	0.41			
1:A:293:LEU:O	1:A:294:GLN:NE2	2.54	0.41			
1:A:331:PHE:O	1:A:331:PHE:CD2	2.74	0.41			
1:A:329:ARG:NH2	1:A:344:LYS:O	2.51	0.41			
1:B:128:LEU:HD12	1:B:128:LEU:HA	1.92	0.41			
1:C:256:CYS:HA	1:C:310:TYR:CD2	2.56	0.41			
1:B:158:LEU:O	1:B:162:MET:HG3	2.21	0.41			
1:B:170:PRO:HG2	1:C:108:ASN:O	2.20	0.41			
1:B:217:ILE:HG22	1:B:218:GLU:H	1.86	0.41			
1:C:128:LEU:O	1:C:131:ALA:HB3	2.21	0.41			
1:C:412:ASN:HB2	1:C:413:ASN:H	1.66	0.41			
1:B:461:ASP:O	1:B:462:ILE:C	2.58	0.41			
1:C:126:PRO:C	1:C:128:LEU:N	2.73	0.41			
1:C:129:LYS:O	1:C:132:LEU:HB2	2.21	0.41			
1:A:260:GLU:O	1:A:260:GLU:CG	2.69	0.41			
1:A:450:ASP:HB3	1:A:453:LYS:HB2	2.03	0.41			
1:B:251:GLU:HG3	1:B:317:SER:HB2	2.02	0.41			
1:B:342:VAL:HG12	1:B:343:LEU:N	2.36	0.41			
1:C:110:GLY:O	1:C:111:ASN:HB2	2.21	0.41			
1:C:139:LEU:O	1:C:139:LEU:HD23	2.21	0.41			
1:C:355:TYR:C	1:C:357:LEU:N	2.74	0.41			
1:B:320:PRO:O	1:B:417:TYR:HE2	2.04	0.40			
1:C:115:MET:O	1:C:118:THR:HB	2.20	0.40			
1:C:457:VAL:CG2	1:C:461:ASP:CG	2.89	0.40			
1:C:181:ALA:O	1:C:182:PHE:CD2	2.74	0.40			
1:C:208:ARG:O	1:C:212:GLN:HG2	2.21	0.40			
1:A:282:VAL:HG13	1:A:287:THR:HB	2.03	0.40			
1:C:438:TRP:CH2	1:C:448:LYS:HE3	2.57	0.40			



Atom-1	Atom-2	${f Interatomic}\ {f distance}\ ({ m \AA})$	Clash overlap (Å)
1:C:442:LYS:O	1:C:443:GLN:C	2.60	0.40
1:C:419:LEU:HD13	1:C:479:TYR:CZ	2.57	0.40
1:B:438:TRP:CH2	1:B:448:LYS:HE3	2.56	0.40
1:B:446:TRP:CG	1:B:462:ILE:HD11	2.57	0.40
1:A:316:ILE:HG13	1:A:357:LEU:O	2.21	0.40
1:B:115:MET:O	1:B:118:THR:HB	2.21	0.40
1:C:135:TYR:CG	1:C:136:ALA:N	2.89	0.40
1:C:184:GLN:HG2	1:C:185:PHE:N	2.36	0.40
1:C:203:TRP:C	1:C:203:TRP:CD1	2.95	0.40
1:C:455:SER:OG	1:C:456:ILE:N	2.55	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	Pe	erce	entiles
1	А	329/404~(81%)	231 (70%)	74 (22%)	24 (7%)		1	7
1	В	329/404~(81%)	233 (71%)	73 (22%)	23 (7%)		1	8
1	С	329/404~(81%)	232~(70%)	74 (22%)	23 (7%)		1	8
All	All	987/1212 (81%)	696 (70%)	221 (22%)	70 (7%)		1	8

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	165	THR
1	А	259	SER
1	А	337	SER
1	А	369	PHE
1	А	370	ARG
1	А	402	PRO
1	А	405	PHE



Mol	Chain	Res	Type
1	В	165	THR
1	В	259	SER
1	В	280	GLN
1	В	337	SER
1	В	370	ARG
1	В	402	PRO
1	В	405	PHE
1	С	165	THR
1	С	259	SER
1	С	337	SER
1	С	356	GLU
1	С	370	ARG
1	С	402	PRO
1	С	405	PHE
1	А	260	GLU
1	А	280	GLN
1	А	356	GLU
1	А	372	LYS
1	А	411	SER
1	А	419	LEU
1	В	127	GLU
1	В	260	GLU
1	В	356	GLU
1	В	411	SER
1	С	110	GLY
1	С	260	GLU
1	С	280	GLN
1	С	419	LEU
1	A	451	ASP
1	A	455	SER
1	В	126	PRO
1	В	369	PHE
1	В	372	LYS
1	B	375	ASP
1	В	419	LEU
1	B	455	SER
1	С	126	PRO
1	С	328	VAL
1	C	369	PHE
1	С	411	SER
1	A	257	THR
1	A	258	GLU



Mol	Chain	Res	Type
1	А	375	ASP
1	В	138	ALA
1	В	444	ASP
1	В	451	ASP
1	С	372	LYS
1	С	375	ASP
1	C	413	ASN
1	С	451	ASP
1	А	138	ALA
1	А	410	GLY
1	А	413	ASN
1	В	110	GLY
1	С	127	GLU
1	С	138	ALA
1	В	410	GLY
1	С	410	GLY
1	В	338	VAL
1	A	126	PRO
1	A	209	VAL
1	С	338	VAL
1	А	338	VAL

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	Perc	entiles
1	А	303/363~(84%)	279~(92%)	24 (8%)	12	43
1	В	303/363~(84%)	280~(92%)	23 (8%)	13	45
1	С	303/363~(84%)	275~(91%)	28 (9%)	9	33
All	All	909/1089~(84%)	834 (92%)	75 (8%)	11	40

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	123	ARG
	a .:	7	



Mol	Chain	Res	Type
1	А	156	ARG
1	A	184	GLN
1	A	265	THR
1	A	276	CYS
1	A	279	ASN
1	A	291	LEU
1	А	292	ARG
1	A	309	LEU
1	A	318	ARG
1	A	324	THR
1	A	331	PHE
1	A	343	LEU
1	A	375	ASP
1	A	402	PRO
1	А	404	SER
1	A	405	PHE
1	А	408	ASP
1	А	412	ASN
1	А	416	TYR
1	А	418	ASP
1	A	423	LEU
1	А	478	LEU
1	А	482	ARG
1	В	123	ARG
1	В	156	ARG
1	В	158	LEU
1	В	184	GLN
1	В	265	THR
1	В	276	CYS
1	В	291	LEU
1	В	292	ARG
1	В	318	ARG
1	В	320	PRO
1	В	324	THR
1	В	331	PHE
1	В	375	ASP
1	В	402	PRO
1	В	405	PHE
1	В	408	ASP
1	В	412	ASN
1	В	416	TYR
1	В	418	ASP



Mol	Chain	Res	Type
1	В	423	LEU
1	В	475	TYR
1	В	478	LEU
1	В	482	ARG
1	С	123	ARG
1	С	156	ARG
1	С	158	LEU
1	С	184	GLN
1	С	265	THR
1	С	276	CYS
1	С	291	LEU
1	С	292	ARG
1	С	318	ARG
1	С	320	PRO
1	С	324	THR
1	С	331	PHE
1	С	332	TYR
1	С	334	GLU
1	С	336	GLU
1	С	343	LEU
1	С	375	ASP
1	С	402	PRO
1	С	404	SER
1	С	405	PHE
1	С	408	ASP
1	С	411	SER
1	С	412	ASN
1	С	416	TYR
1	C	418	ASP
1	С	423	LEU
1	С	478	LEU
1	С	482	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	120	GLN
1	А	149	GLN
1	А	176	GLN
1	А	184	GLN
1	А	191	GLN
1	А	200	ASN



Mol	Chain	Res	Type
1	А	205	GLN
1	А	273	GLN
1	А	326	GLN
1	А	412	ASN
1	В	149	GLN
1	В	176	GLN
1	В	184	GLN
1	В	200	ASN
1	В	205	GLN
1	В	271	GLN
1	В	273	GLN
1	В	294	GLN
1	В	326	GLN
1	В	412	ASN
1	С	120	GLN
1	С	149	GLN
1	С	176	GLN
1	С	184	GLN
1	С	205	GLN
1	С	271	GLN
1	С	273	GLN
1	C	294	GLN
1	С	326	GLN
1	C	412	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

