



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:01 am BST

PDB ID : 2DZO  
Title : Crystal structure analysis of yeast Nas6p complexed with the proteasome subunit, rpt3  
Authors : Nakamura, Y.; Padmanabhan, B.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-09-29  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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

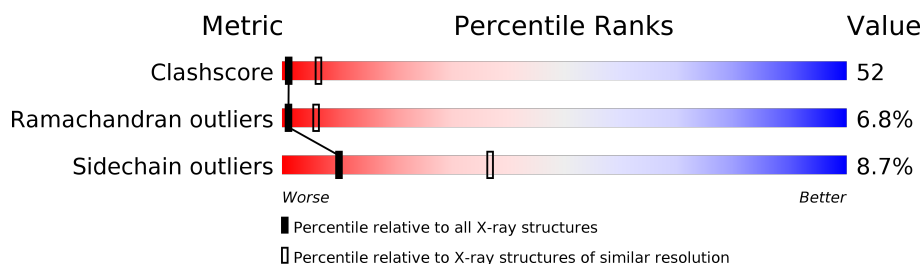
# 1 Overall quality at a glance

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	228	<div> <div>32%</div> <div>58%</div> <div>9%</div> </div>
1	C	228	<div> <div>35%</div> <div>60%</div> <div>5%</div> </div>
2	B	82	<div> <div>20%</div> <div>39%</div> <div>10%</div> <div>•</div> <div>30%</div> </div>
2	D	82	<div> <div>26%</div> <div>39%</div> <div>13%</div> <div>•</div> <div>18%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4763 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 Probable 26S proteasome regulatory subunit p28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1808	1159	307	335	7			
1	C	227	Total	C	N	O	S	0	0	0
			1800	1154	306	334	6			

- Molecule 2 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	57	Total	C	N	O	S	0	0	0
			434	270	76	86	2			
2	D	67	Total	C	N	O	S	0	0	0
			515	321	92	100	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	347	MET	-	INITIATING METHIONINE	UNP P33298
D	347	MET	-	INITIATING METHIONINE	UNP P33298

- Molecule 3 is water.

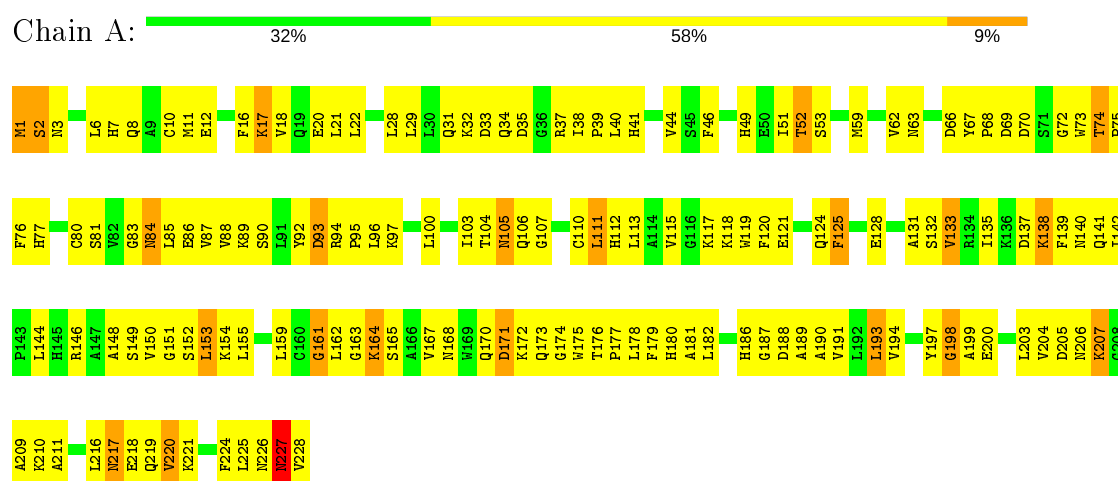
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	13	Total	O	0	0
			13	13		
3	C	92	Total	O	0	0
			92	92		
3	D	15	Total	O	0	0
			15	15		

### 3 Residue-property plots

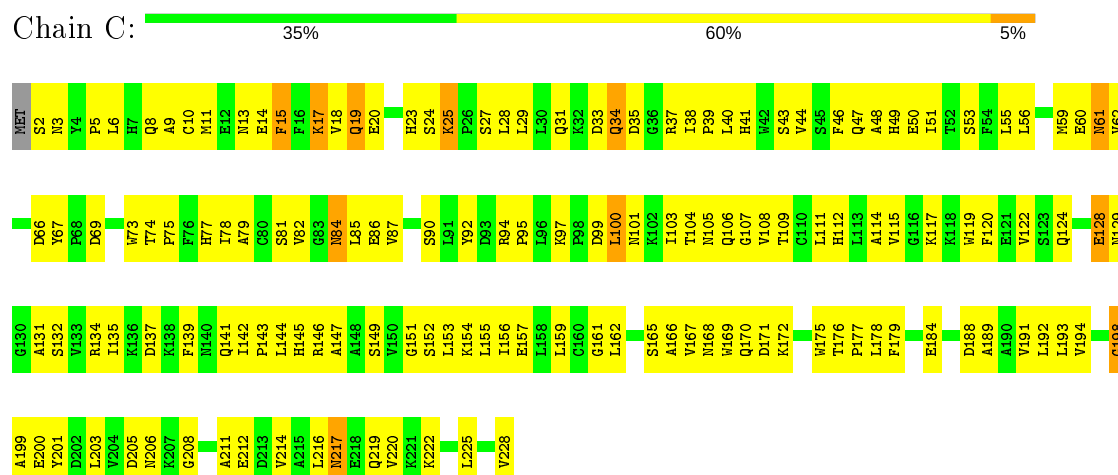
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

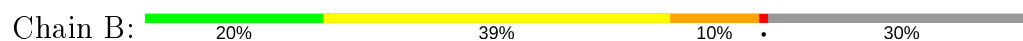
- Molecule 1: Probable 26S proteasome regulatory subunit p28

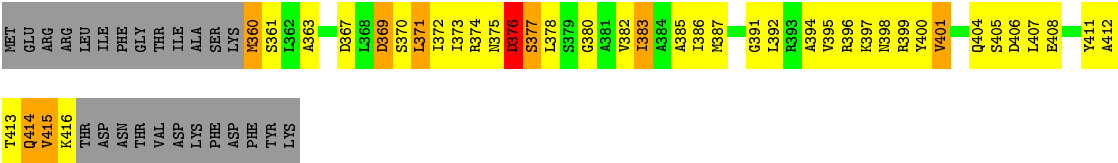


- Molecule 1: Probable 26S proteasome regulatory subunit p28

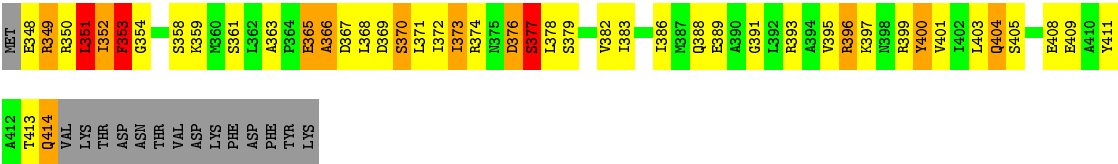
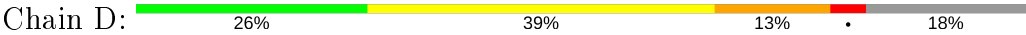


- Molecule 2: 26S protease regulatory subunit 6B homolog





• Molecule 2: 26S protease regulatory subunit 6B homolog



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.60 Å 99.60 Å 73.08 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	96.0 (20.00-3.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.212 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.39	0/1851	0.64	0/2506
1	C	0.38	0/1843	0.62	0/2496
2	B	0.41	0/436	0.68	0/588
2	D	0.36	0/518	0.69	0/697
All	All	0.38	0/4648	0.64	0/6287

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	A	1808	0	1792	165	0
1	C	1800	0	1780	189	0
2	B	434	0	447	62	0
2	D	515	0	532	72	0
3	A	86	0	0	12	1
3	B	13	0	0	1	1
3	C	92	0	0	26	0
3	D	15	0	0	9	0
All	All	4763	0	4551	470	1

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 52.

All (470) 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:A:210:LYS:HG3	3:A:238:HOH:O	1.21	1.28
1:A:17:LYS:NZ	1:A:21:LEU:HD11	1.44	1.27
2:D:359:LYS:HB2	3:D:438:HOH:O	1.29	1.25
1:C:15:PHE:CE2	1:C:19:GLN:OE1	1.88	1.25
1:C:151:GLY:HA3	3:C:295:HOH:O	1.10	1.25
1:C:59:MET:HE1	3:C:320:HOH:O	1.44	1.16
1:C:114:ALA:HB1	3:C:270:HOH:O	1.53	1.09
1:C:78:ILE:HG23	2:D:365:GLU:HG2	1.38	1.05
3:A:295:HOH:O	2:B:375:ASN:HB2	1.59	1.00
1:A:142:ILE:HD12	3:A:314:HOH:O	1.61	0.98
1:C:66:ASP:HB3	3:C:306:HOH:O	1.64	0.97
1:C:74:THR:H	1:C:77:HIS:HD2	1.17	0.93
1:A:168:ASN:HD21	1:A:200:GLU:H	1.17	0.93
2:B:367:ASP:HB3	2:B:404:GLN:HE21	1.35	0.92
1:A:17:LYS:HZ3	1:A:21:LEU:HD11	1.05	0.92
2:D:359:LYS:HD3	2:D:359:LYS:O	1.67	0.92
1:A:17:LYS:NZ	1:A:21:LEU:CD1	2.34	0.91
1:C:151:GLY:CA	3:C:295:HOH:O	1.82	0.90
1:A:17:LYS:HZ1	1:A:21:LEU:HD21	1.35	0.90
1:A:40:LEU:O	1:A:44:VAL:HG23	1.73	0.89
2:B:394:ALA:HA	2:B:399:ARG:HH21	1.37	0.89
1:C:53:SER:O	3:C:232:HOH:O	1.91	0.87
1:C:15:PHE:CZ	1:C:19:GLN:OE1	2.28	0.87
1:A:153:LEU:HD22	1:A:153:LEU:H	1.40	0.87
1:A:93:ASP:OD1	3:A:249:HOH:O	1.95	0.85
2:D:349:ARG:NH1	2:D:350:ARG:H	1.75	0.85
1:C:47:GLN:HE21	1:C:84:ASN:HB2	1.39	0.84
1:C:119:TRP:HB2	3:C:270:HOH:O	1.77	0.83
1:C:194:VAL:O	1:C:198:GLY:HA2	1.79	0.83
2:B:377:SER:HA	2:D:359:LYS:NZ	1.93	0.83
1:C:219:GLN:NE2	3:C:229:HOH:O	1.84	0.82
1:C:74:THR:H	1:C:77:HIS:CD2	1.96	0.82
1:A:225:LEU:HD22	1:A:225:LEU:H	1.46	0.81
1:C:8:GLN:HG3	3:C:238:HOH:O	1.80	0.81
1:A:111:LEU:HD12	1:A:115:VAL:HG23	1.65	0.79
1:A:17:LYS:HZ1	1:A:21:LEU:HD11	1.44	0.78
1:A:217:ASN:ND2	1:A:220:VAL:H	1.81	0.78
1:A:38:ILE:H	1:A:41:HIS:HD2	1.28	0.78
1:C:108:VAL:HA	3:C:268:HOH:O	1.82	0.78
1:A:74:THR:HG23	1:A:76:PHE:H	1.48	0.78

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ASN:H	1:C:61:ASN:HD22	1.29	0.78
1:A:146:ARG:HH22	2:B:370:SER:HB3	1.49	0.78
2:D:368:LEU:O	2:D:372:ILE:HG13	1.82	0.77
1:C:44:VAL:HG13	1:C:87:VAL:HG11	1.65	0.77
2:D:376:ASP:O	3:D:431:HOH:O	2.02	0.77
1:C:217:ASN:HD21	1:C:220:VAL:HG23	1.49	0.77
1:C:38:ILE:H	1:C:41:HIS:HD2	1.30	0.77
1:A:168:ASN:HD21	1:A:200:GLU:N	1.82	0.76
1:A:17:LYS:HZ1	1:A:21:LEU:CD2	1.99	0.75
1:C:144:LEU:HD23	1:C:177:PRO:HG2	1.68	0.74
1:A:103:ILE:HB	1:A:107:GLY:HA2	1.69	0.74
1:C:15:PHE:HE2	1:C:19:GLN:CG	1.99	0.74
2:D:349:ARG:NH1	2:D:350:ARG:N	2.35	0.74
2:B:361:SER:HB3	1:C:216:LEU:HD21	1.68	0.74
1:C:152:SER:OG	1:C:155:LEU:HD23	1.88	0.73
2:D:379:SER:O	2:D:382:VAL:HG12	1.88	0.73
2:D:358:SER:HA	3:D:437:HOH:O	1.88	0.73
2:D:377:SER:HB2	3:D:431:HOH:O	1.88	0.73
1:C:112:HIS:CE1	1:C:143:PRO:HD3	2.24	0.73
1:A:137:ASP:O	1:A:139:PHE:N	2.23	0.72
1:C:15:PHE:HE2	1:C:19:GLN:HG2	1.55	0.72
1:C:78:ILE:O	1:C:82:VAL:HG23	1.90	0.72
1:C:15:PHE:CE2	1:C:19:GLN:CD	2.62	0.71
1:A:73:TRP:CZ2	2:B:404:GLN:HG3	2.25	0.71
2:B:371:LEU:HD21	2:B:411:TYR:CD1	2.25	0.71
2:B:391:GLY:O	2:B:395:VAL:HG23	1.90	0.71
1:C:100:LEU:HD13	1:C:131:ALA:HB2	1.73	0.71
2:D:400:TYR:CD1	2:D:401:VAL:HG23	2.26	0.70
1:A:111:LEU:O	1:A:115:VAL:HG23	1.90	0.70
1:A:217:ASN:C	1:A:217:ASN:HD22	1.95	0.70
1:C:107:GLY:O	1:C:137:ASP:HA	1.92	0.70
2:D:367:ASP:OD1	2:D:369:ASP:HB2	1.91	0.70
1:A:104:THR:O	1:A:107:GLY:N	2.24	0.70
1:A:31:GLN:O	1:A:38:ILE:HA	1.92	0.69
1:A:17:LYS:CE	1:A:21:LEU:HD11	2.22	0.69
1:A:148:ALA:HB1	1:A:181:ALA:HB2	1.74	0.68
1:C:44:VAL:HG11	1:C:79:ALA:HB2	1.76	0.68
1:A:6:LEU:CD2	1:A:28:LEU:HB3	2.23	0.68
1:C:29:LEU:O	3:C:320:HOH:O	2.12	0.67
2:B:372:ILE:HG13	2:B:373:ILE:N	2.09	0.67
3:A:295:HOH:O	2:B:375:ASN:CB	2.30	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:367:ASP:H	2:D:404:GLN:HE21	1.41	0.67
1:C:15:PHE:HE2	1:C:19:GLN:OE1	1.71	0.67
2:B:404:GLN:HA	2:B:407:LEU:HD12	1.76	0.66
2:B:396:ARG:HG2	2:B:396:ARG:HH11	1.61	0.66
1:C:74:THR:N	1:C:77:HIS:HD2	1.92	0.66
1:C:194:VAL:HA	1:C:199:ALA:H	1.60	0.66
2:D:349:ARG:HH11	2:D:350:ARG:N	1.94	0.66
1:C:61:ASN:N	1:C:61:ASN:HD22	1.89	0.65
1:A:74:THR:CG2	1:A:76:PHE:H	2.10	0.65
1:C:104:THR:OG1	1:C:108:VAL:HG22	1.95	0.65
2:B:367:ASP:HB3	2:B:404:GLN:NE2	2.09	0.65
1:A:152:SER:OG	1:A:155:LEU:HD23	1.97	0.65
2:B:367:ASP:OD2	2:B:370:SER:HB3	1.96	0.65
2:B:394:ALA:HA	2:B:399:ARG:NH2	2.10	0.65
1:A:133:VAL:HG13	1:A:133:VAL:O	1.96	0.65
1:C:15:PHE:CE2	1:C:19:GLN:CG	2.80	0.65
1:C:217:ASN:ND2	1:C:220:VAL:H	1.95	0.64
1:A:6:LEU:HD23	1:A:28:LEU:HB3	1.78	0.64
1:C:141:GLN:HG2	1:C:171:ASP:HB3	1.79	0.64
2:B:413:THR:O	2:B:414:GLN:HG2	1.98	0.64
1:C:25:LYS:O	1:C:25:LYS:HG3	1.97	0.64
1:C:61:ASN:ND2	1:C:61:ASN:N	2.45	0.64
1:C:146:ARG:NE	3:C:269:HOH:O	2.31	0.64
1:C:172:LYS:HE3	3:C:291:HOH:O	1.96	0.64
1:C:73:TRP:CZ2	2:D:404:GLN:HG3	2.33	0.63
2:D:376:ASP:HA	3:D:443:HOH:O	1.99	0.63
2:B:377:SER:HA	2:D:359:LYS:HZ1	1.62	0.63
2:B:367:ASP:CB	2:B:404:GLN:HE21	2.10	0.63
1:C:40:LEU:O	1:C:44:VAL:HG23	1.98	0.63
1:C:134:ARG:NH1	1:C:166:ALA:HB2	2.14	0.62
1:C:134:ARG:HH12	1:C:166:ALA:HB2	1.64	0.62
2:B:415:VAL:HG12	2:B:416:LYS:N	2.14	0.62
1:C:56:LEU:HD21	1:C:94:ARG:HD2	1.82	0.61
2:D:349:ARG:HH11	2:D:351:LEU:N	1.98	0.61
1:C:103:ILE:HB	1:C:107:GLY:HA2	1.80	0.61
1:A:133:VAL:CG2	1:A:159:LEU:HD23	2.29	0.61
1:C:175:TRP:CE3	1:C:179:PHE:HB3	2.34	0.61
1:A:17:LYS:HZ1	1:A:21:LEU:CD1	2.05	0.61
1:A:194:VAL:HA	1:A:199:ALA:H	1.65	0.61
2:D:399:ARG:NH1	2:D:403:LEU:HG	2.16	0.61
1:C:201:TYR:CE2	1:C:228:VAL:HB	2.35	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PHE:HE1	1:A:205:ASP:HB3	1.66	0.60
1:C:153:LEU:HD12	1:C:153:LEU:H	1.67	0.60
2:B:377:SER:HA	2:D:359:LYS:HZ2	1.66	0.60
2:D:376:ASP:C	3:D:431:HOH:O	2.38	0.60
1:C:38:ILE:N	1:C:41:HIS:HD2	2.00	0.59
1:C:15:PHE:HE2	1:C:19:GLN:CD	2.02	0.59
1:C:178:LEU:HA	1:C:193:LEU:CD1	2.32	0.59
1:A:146:ARG:NH2	2:B:370:SER:HB3	2.17	0.59
1:A:153:LEU:CD2	1:A:153:LEU:H	2.13	0.59
1:A:133:VAL:HG22	1:A:159:LEU:HD23	1.84	0.59
2:D:400:TYR:HD1	2:D:401:VAL:HG23	1.66	0.59
1:A:206:ASN:O	1:A:207:LYS:HG3	2.01	0.59
2:D:391:GLY:O	2:D:395:VAL:HG23	2.03	0.58
1:C:168:ASN:HD21	1:C:200:GLU:H	1.51	0.58
1:A:74:THR:HB	1:A:77:HIS:HD2	1.69	0.58
2:B:360:MET:N	2:B:360:MET:SD	2.77	0.58
1:C:169:TRP:O	1:C:176:THR:HA	2.03	0.58
2:B:360:MET:HG2	2:B:361:SER:H	1.68	0.58
1:C:56:LEU:HB3	3:C:232:HOH:O	2.02	0.58
1:A:76:PHE:CE1	1:A:88:VAL:HG13	2.39	0.58
1:C:69:ASP:OD2	1:C:73:TRP:HB2	2.03	0.58
1:A:153:LEU:CD1	1:A:189:ALA:HA	2.34	0.57
1:C:135:ILE:HD12	1:C:135:ILE:H	1.69	0.57
1:C:162:LEU:HD23	1:C:162:LEU:C	2.25	0.57
1:A:74:THR:O	1:A:77:HIS:N	2.37	0.57
1:C:212:GLU:OE1	1:C:225:LEU:HD21	2.04	0.57
1:A:140:ASN:HB2	1:A:171:ASP:HA	1.86	0.57
1:A:140:ASN:ND2	1:A:172:LYS:HE3	2.19	0.56
2:D:378:LEU:HB3	2:D:382:VAL:CG1	2.35	0.56
1:C:8:GLN:C	1:C:10:CYS:H	2.08	0.56
1:A:135:ILE:HA	3:A:235:HOH:O	2.05	0.56
1:A:170:GLN:HG2	1:A:176:THR:HG23	1.87	0.56
1:A:20:GLU:HG3	3:A:313:HOH:O	2.05	0.56
2:B:371:LEU:HD21	2:B:411:TYR:CG	2.41	0.56
1:C:73:TRP:HA	1:C:77:HIS:CD2	2.41	0.56
2:D:365:GLU:O	2:D:366:ALA:C	2.43	0.56
1:C:200:GLU:HB2	1:C:203:LEU:HD11	1.88	0.56
1:A:137:ASP:C	1:A:139:PHE:H	2.09	0.56
1:C:43:SER:HB3	3:C:245:HOH:O	2.05	0.55
1:A:74:THR:H	1:A:77:HIS:HB2	1.71	0.55
2:D:348:GLU:N	2:D:376:ASP:HB3	2.22	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:CB	3:C:306:HOH:O	2.34	0.55
1:C:38:ILE:H	1:C:41:HIS:CD2	2.19	0.55
2:B:378:LEU:HB3	2:B:383:ILE:CD1	2.36	0.55
1:C:189:ALA:O	1:C:192:LEU:HB3	2.07	0.55
1:A:204:VAL:HA	1:A:209:ALA:O	2.07	0.55
1:C:105:ASN:HB3	1:C:106:GLN:NE2	2.23	0.54
1:C:217:ASN:ND2	1:C:219:GLN:HB3	2.22	0.54
1:C:67:TYR:O	1:C:75:PRO:HD3	2.06	0.54
2:D:395:VAL:C	2:D:397:LYS:H	2.10	0.54
1:A:144:LEU:HA	1:A:159:LEU:HD13	1.88	0.54
1:C:8:GLN:C	1:C:10:CYS:N	2.59	0.54
1:A:7:HIS:CD2	1:A:39:PRO:HG3	2.42	0.54
2:B:371:LEU:CD2	2:B:411:TYR:CD1	2.90	0.54
1:A:217:ASN:ND2	1:A:220:VAL:HG23	2.22	0.54
1:A:76:PHE:HE1	1:A:88:VAL:HG13	1.73	0.54
1:C:166:ALA:HB1	1:C:169:TRP:NE1	2.23	0.54
1:A:74:THR:HG22	1:A:77:HIS:H	1.72	0.54
1:C:61:ASN:ND2	1:C:61:ASN:H	1.98	0.54
1:A:226:ASN:O	1:A:227:ASN:HB2	2.08	0.53
2:D:371:LEU:HD22	2:D:411:TYR:CG	2.43	0.53
1:C:56:LEU:CD2	1:C:94:ARG:HD2	2.38	0.53
2:B:411:TYR:O	2:B:415:VAL:HG23	2.09	0.53
1:A:133:VAL:HG22	1:A:159:LEU:CD2	2.39	0.53
1:C:132:SER:HB3	1:C:135:ILE:HD11	1.90	0.53
1:A:217:ASN:HD21	1:A:220:VAL:H	1.54	0.53
1:A:163:GLY:O	1:A:164:LYS:C	2.47	0.53
1:C:135:ILE:N	1:C:135:ILE:HD12	2.25	0.52
1:A:6:LEU:CD1	1:A:18:VAL:HG13	2.39	0.52
1:A:18:VAL:HG21	1:A:51:ILE:HD13	1.90	0.52
1:C:170:GLN:HG2	1:C:176:THR:HG23	1.92	0.52
1:A:121:GLU:HB2	3:A:300:HOH:O	2.10	0.52
1:A:188:ASP:O	1:A:191:VAL:HG22	2.09	0.52
2:B:396:ARG:C	2:B:398:ASN:H	2.13	0.52
1:A:152:SER:OG	1:A:155:LEU:HB2	2.10	0.52
1:A:6:LEU:HD11	1:A:18:VAL:HG13	1.92	0.52
1:C:146:ARG:NH2	3:C:269:HOH:O	2.43	0.52
1:C:2:SER:O	1:C:3:ASN:C	2.47	0.52
2:D:396:ARG:O	2:D:396:ARG:HG3	2.10	0.52
1:C:159:LEU:O	1:C:165:SER:HB2	2.10	0.51
1:A:83:GLY:HA2	1:A:119:TRP:CD1	2.46	0.51
1:C:211:ALA:O	1:C:214:VAL:HG22	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:ARG:HH12	2:D:350:ARG:HB3	1.76	0.51
1:A:161:GLY:O	1:A:164:LYS:HD2	2.10	0.51
1:A:85:LEU:HD11	1:A:89:LYS:HE2	1.92	0.51
2:B:372:ILE:HG13	2:B:373:ILE:H	1.75	0.51
1:A:35:ASP:OD1	2:B:399:ARG:NH1	2.44	0.51
1:C:129:ASN:O	3:C:276:HOH:O	2.19	0.51
1:A:162:LEU:HD23	1:A:162:LEU:C	2.31	0.51
1:A:217:ASN:HD21	1:A:220:VAL:HG23	1.76	0.51
2:D:369:ASP:HA	2:D:372:ILE:HD12	1.93	0.51
1:C:84:ASN:ND2	1:C:86:GLU:HB2	2.25	0.50
2:D:358:SER:CA	3:D:437:HOH:O	2.54	0.50
2:B:380:GLY:C	2:B:383:ILE:HG12	2.32	0.50
1:C:111:LEU:O	1:C:115:VAL:HG23	2.11	0.50
2:D:352:ILE:HB	2:D:383:ILE:HD12	1.94	0.50
1:A:173:GLN:NE2	2:B:375:ASN:HA	2.25	0.50
1:A:32:LYS:HA	1:A:37:ARG:O	2.12	0.50
1:C:62:VAL:HG22	1:C:67:TYR:HE2	1.77	0.50
1:A:125:PHE:C	1:A:125:PHE:CD2	2.85	0.50
1:A:124:GLN:O	1:A:128:GLU:HG3	2.11	0.50
1:C:81:SER:O	1:C:117:LYS:HD2	2.12	0.50
1:A:80:CYS:SG	1:A:110:CYS:HB3	2.52	0.50
1:C:9:ALA:HB2	1:C:17:LYS:HG3	1.92	0.50
2:D:371:LEU:HD22	2:D:411:TYR:HB2	1.92	0.50
1:C:94:ARG:HB3	1:C:95:PRO:HD2	1.93	0.50
2:D:374:ARG:C	2:D:376:ASP:H	2.16	0.50
1:A:179:PHE:CE1	1:A:205:ASP:HB3	2.46	0.49
1:A:17:LYS:HZ1	1:A:21:LEU:CG	2.25	0.49
2:B:396:ARG:HG2	2:B:396:ARG:NH1	2.27	0.49
1:C:31:GLN:O	1:C:38:ILE:HA	2.11	0.49
2:B:387:MET:HG3	2:D:352:ILE:HD13	1.93	0.49
2:B:378:LEU:HD22	2:B:382:VAL:HB	1.94	0.49
1:C:146:ARG:CZ	3:C:269:HOH:O	2.60	0.49
1:C:217:ASN:HD21	1:C:220:VAL:H	1.59	0.49
1:C:99:ASP:O	1:C:101:ASN:N	2.45	0.49
2:B:397:LYS:O	2:B:399:ARG:HG3	2.12	0.49
1:A:167:VAL:O	1:A:177:PRO:HD2	2.11	0.49
1:C:217:ASN:CG	1:C:219:GLN:HB3	2.33	0.49
2:D:374:ARG:HH22	2:D:408:GLU:CD	2.15	0.49
1:C:162:LEU:HD23	1:C:162:LEU:O	2.12	0.49
2:D:349:ARG:CD	2:D:351:LEU:HB2	2.42	0.49
1:A:6:LEU:HD21	1:A:22:LEU:HD21	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:O	1:C:145:HIS:HB2	2.13	0.49
2:B:415:VAL:HG12	2:B:416:LYS:H	1.76	0.48
1:C:167:VAL:HG11	1:C:199:ALA:HB2	1.93	0.48
2:D:363:ALA:HB2	2:D:401:VAL:HG12	1.95	0.48
2:B:363:ALA:HB2	2:B:401:VAL:CG2	2.43	0.48
2:B:394:ALA:CA	2:B:399:ARG:HH21	2.18	0.48
2:D:403:LEU:O	2:D:404:GLN:C	2.51	0.48
1:A:6:LEU:HD22	1:A:28:LEU:HB3	1.94	0.48
1:C:132:SER:HB3	1:C:135:ILE:CD1	2.42	0.48
1:C:175:TRP:CD2	1:C:179:PHE:HB3	2.49	0.48
1:C:94:ARG:HB3	1:C:95:PRO:CD	2.44	0.48
1:A:162:LEU:HD23	1:A:162:LEU:O	2.14	0.48
1:C:41:HIS:ND1	1:C:78:ILE:HD11	2.28	0.48
2:D:371:LEU:HD23	2:D:374:ARG:NH2	2.27	0.48
1:A:186:HIS:O	1:A:189:ALA:N	2.45	0.48
2:B:380:GLY:HA2	2:B:383:ILE:CG1	2.44	0.48
1:A:217:ASN:HD22	1:A:220:VAL:H	1.60	0.48
2:B:369:ASP:OD1	2:B:369:ASP:N	2.36	0.48
2:B:382:VAL:HG12	2:B:386:ILE:CD1	2.44	0.48
1:A:111:LEU:HD12	1:A:115:VAL:CG2	2.40	0.48
1:C:166:ALA:CB	1:C:169:TRP:CE2	2.97	0.48
2:D:396:ARG:HD2	3:D:435:HOH:O	2.13	0.48
2:B:399:ARG:NH2	2:B:406:ASP:OD2	2.47	0.48
1:C:115:VAL:CG1	1:C:147:ALA:HB2	2.43	0.48
1:C:167:VAL:CG1	1:C:199:ALA:HB2	2.44	0.48
2:D:376:ASP:HB3	3:D:431:HOH:O	2.14	0.48
2:B:375:ASN:O	2:B:376:ASP:C	2.52	0.47
1:C:2:SER:O	1:C:5:PRO:HD3	2.12	0.47
1:C:33:ASP:O	1:C:35:ASP:N	2.47	0.47
1:C:170:GLN:HG2	1:C:176:THR:CG2	2.44	0.47
1:A:188:ASP:N	1:A:188:ASP:OD1	2.48	0.47
1:C:168:ASN:ND2	1:C:200:GLU:H	2.11	0.47
2:B:399:ARG:HH22	2:B:406:ASP:CG	2.18	0.47
1:C:103:ILE:HD12	1:C:107:GLY:HA2	1.97	0.47
1:C:87:VAL:O	1:C:90:SER:HB3	2.15	0.47
1:A:225:LEU:HA	1:A:228:VAL:HG22	1.97	0.47
1:C:86:GLU:OE1	1:C:86:GLU:HA	2.14	0.47
2:D:351:LEU:O	2:D:352:ILE:C	2.51	0.47
1:A:117:LYS:O	1:A:118:LYS:HB2	2.15	0.47
1:A:69:ASP:OD2	1:A:73:TRP:HB2	2.15	0.47
1:C:179:PHE:CE1	1:C:205:ASP:HB3	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:N	1:A:77:HIS:HB2	2.31	0.47
2:B:383:ILE:N	2:B:383:ILE:HD13	2.30	0.47
1:C:38:ILE:HD12	3:C:320:HOH:O	2.14	0.46
2:D:379:SER:O	2:D:383:ILE:HG13	2.15	0.46
1:A:182:LEU:HD12	1:A:211:ALA:HB1	1.98	0.46
2:B:411:TYR:CE1	2:B:415:VAL:HG21	2.49	0.46
1:C:59:MET:C	1:C:61:ASN:H	2.17	0.46
1:A:17:LYS:HZ3	1:A:21:LEU:CD1	1.98	0.46
1:A:74:THR:H	1:A:77:HIS:CD2	2.33	0.46
1:C:217:ASN:N	1:C:217:ASN:HD22	2.14	0.46
1:C:47:GLN:HE21	1:C:84:ASN:CB	2.19	0.46
1:C:105:ASN:HB3	1:C:106:GLN:HE22	1.80	0.46
1:C:34:GLN:O	2:D:397:LYS:HE2	2.16	0.46
2:D:353:PHE:O	2:D:354:GLY:C	2.52	0.46
1:C:120:PHE:HD1	1:C:155:LEU:HD22	1.79	0.46
1:C:205:ASP:C	1:C:205:ASP:OD2	2.54	0.46
2:D:370:SER:OG	2:D:374:ARG:NH2	2.42	0.46
1:A:146:ARG:NH1	3:A:288:HOH:O	2.48	0.46
2:D:373:ILE:HG13	2:D:373:ILE:O	2.15	0.46
2:D:371:LEU:HD23	2:D:374:ARG:CZ	2.45	0.46
1:A:11:MET:HA	1:A:46:PHE:CD2	2.51	0.46
2:B:374:ARG:HH22	2:B:408:GLU:CD	2.19	0.46
1:C:24:SER:O	1:C:25:LYS:HB3	2.15	0.46
1:A:37:ARG:HA	1:A:41:HIS:CD2	2.51	0.46
1:C:217:ASN:C	1:C:217:ASN:HD22	2.18	0.46
1:C:73:TRP:HA	1:C:77:HIS:HD2	1.80	0.46
1:C:167:VAL:O	1:C:167:VAL:HG12	2.16	0.46
1:C:15:PHE:CE2	1:C:19:GLN:HG2	2.43	0.46
1:A:1:MET:O	1:A:3:ASN:N	2.49	0.45
1:A:63:ASN:HB3	1:A:66:ASP:OD2	2.15	0.45
1:A:68:PRO:HB2	1:A:72:GLY:HA2	1.99	0.45
1:C:109:THR:O	1:C:112:HIS:HB2	2.17	0.45
1:C:50:GLU:HG3	1:C:51:ILE:H	1.79	0.45
1:C:51:ILE:O	1:C:55:LEU:HG	2.16	0.45
1:C:115:VAL:HG11	1:C:147:ALA:HB2	1.97	0.45
1:C:17:LYS:HD3	1:C:17:LYS:O	2.16	0.45
2:D:397:LYS:HD3	2:D:399:ARG:HH21	1.82	0.45
1:A:38:ILE:H	1:A:41:HIS:CD2	2.19	0.45
1:C:225:LEU:HA	1:C:228:VAL:HG22	1.99	0.45
1:C:84:ASN:C	1:C:84:ASN:HD22	2.19	0.45
1:C:84:ASN:O	1:C:87:VAL:N	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD12	1:A:111:LEU:O	2.17	0.45
1:A:33:ASP:C	1:A:35:ASP:H	2.20	0.45
1:A:74:THR:HG22	1:A:77:HIS:N	2.31	0.45
2:D:414:GLN:HB3	2:D:414:GLN:HE21	1.66	0.45
1:A:7:HIS:HD2	1:A:39:PRO:HG3	1.82	0.45
2:B:373:ILE:O	2:B:373:ILE:CG2	2.64	0.45
1:C:84:ASN:O	1:C:85:LEU:C	2.54	0.45
1:A:67:TYR:O	1:A:75:PRO:HD3	2.17	0.45
1:C:25:LYS:HE2	1:C:28:LEU:CD1	2.47	0.45
2:D:389:GLU:OE2	2:D:389:GLU:HA	2.17	0.44
1:A:100:LEU:HG	3:A:271:HOH:O	2.16	0.44
1:A:49:HIS:HD2	1:A:86:GLU:OE2	2.00	0.44
1:A:149:SER:OG	2:B:373:ILE:HG12	2.17	0.44
1:C:11:MET:HA	1:C:46:PHE:CD2	2.51	0.44
1:C:14:GLU:O	1:C:17:LYS:HB3	2.17	0.44
1:C:139:PHE:O	1:C:171:ASP:HB2	2.17	0.44
1:C:28:LEU:O	1:C:29:LEU:C	2.55	0.44
2:D:374:ARG:NH1	2:D:411:TYR:CD2	2.86	0.44
1:A:133:VAL:HG11	1:A:165:SER:HB2	1.99	0.44
1:A:218:GLU:HA	1:A:218:GLU:OE2	2.18	0.44
2:B:392:LEU:N	2:B:392:LEU:HD12	2.32	0.44
1:C:33:ASP:C	1:C:35:ASP:H	2.20	0.44
2:D:367:ASP:O	2:D:404:GLN:NE2	2.50	0.44
1:A:12:GLU:OE2	1:C:222:LYS:NZ	2.41	0.44
1:A:1:MET:O	1:A:2:SER:C	2.55	0.44
1:A:168:ASN:ND2	1:A:200:GLU:H	1.99	0.44
1:A:216:LEU:HB3	1:A:220:VAL:HG21	2.00	0.44
1:A:92:TYR:O	1:A:97:LYS:HG2	2.17	0.44
2:D:413:THR:O	2:D:413:THR:HG22	2.17	0.44
1:A:175:TRP:CD1	1:A:179:PHE:HD1	2.35	0.44
1:C:2:SER:HB2	3:C:237:HOH:O	2.17	0.44
1:C:18:VAL:HG21	1:C:51:ILE:HD13	2.00	0.44
1:A:200:GLU:OE2	1:A:203:LEU:HD11	2.18	0.44
1:A:40:LEU:HB2	1:A:59:MET:HE1	1.99	0.44
1:C:144:LEU:CD2	1:C:177:PRO:HG2	2.43	0.44
1:C:25:LYS:HE2	1:C:27:SER:OG	2.18	0.44
2:D:349:ARG:HH11	2:D:351:LEU:H	1.65	0.44
1:A:146:ARG:NH2	2:B:367:ASP:OD2	2.51	0.43
1:C:143:PRO:O	1:C:146:ARG:N	2.51	0.43
1:A:172:LYS:C	1:A:174:GLY:H	2.21	0.43
1:A:179:PHE:CD2	1:A:211:ALA:HB2	2.53	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:SER:O	1:C:184:GLU:HG3	2.18	0.43
1:A:87:VAL:O	1:A:90:SER:HB2	2.18	0.43
2:D:393:ARG:HD3	2:D:409:GLU:HG3	2.00	0.43
1:A:112:HIS:O	1:A:113:LEU:C	2.56	0.43
1:A:178:LEU:HD11	1:A:190:ALA:HB1	2.01	0.43
1:C:122:VAL:HG23	3:C:272:HOH:O	2.18	0.43
1:C:8:GLN:O	1:C:10:CYS:N	2.52	0.43
2:D:365:GLU:H	2:D:365:GLU:HG3	1.57	0.43
2:D:348:GLU:OE1	2:D:373:ILE:HG22	2.19	0.43
1:A:81:SER:O	1:A:117:LYS:HD2	2.19	0.43
1:A:217:ASN:C	1:A:217:ASN:ND2	2.68	0.43
2:D:382:VAL:O	2:D:386:ILE:HG13	2.18	0.43
1:C:217:ASN:ND2	1:C:217:ASN:O	2.49	0.43
1:C:59:MET:O	1:C:62:VAL:HG12	2.18	0.43
2:B:380:GLY:CA	2:B:383:ILE:HG12	2.49	0.43
2:B:415:VAL:O	2:B:416:LYS:C	2.57	0.43
1:C:103:ILE:HA	1:C:108:VAL:O	2.19	0.43
1:C:168:ASN:HD21	1:C:200:GLU:N	2.16	0.43
1:A:7:HIS:O	1:A:10:CYS:HB2	2.18	0.42
1:A:132:SER:HB3	1:A:135:ILE:HG13	2.01	0.42
1:A:84:ASN:OD1	1:A:87:VAL:HG23	2.19	0.42
1:A:141:GLN:HG2	1:A:171:ASP:HB3	2.01	0.42
2:B:375:ASN:O	2:B:377:SER:N	2.53	0.42
2:B:378:LEU:HB3	2:B:383:ILE:HD11	1.99	0.42
1:C:217:ASN:ND2	1:C:217:ASN:N	2.67	0.42
2:D:400:TYR:CE1	2:D:401:VAL:HG23	2.53	0.42
1:C:206:ASN:HA	1:C:206:ASN:HD22	1.62	0.42
1:A:203:LEU:N	1:A:203:LEU:HD12	2.35	0.42
1:A:221:LYS:O	1:A:224:PHE:HB3	2.20	0.42
2:B:399:ARG:NH2	2:B:406:ASP:OD1	2.52	0.42
1:C:200:GLU:HB2	1:C:203:LEU:CD1	2.50	0.42
1:C:41:HIS:ND1	1:C:78:ILE:CD1	2.83	0.42
1:C:48:ALA:HB1	1:C:50:GLU:HG3	2.02	0.42
1:A:180:HIS:C	1:A:182:LEU:H	2.23	0.42
1:A:59:MET:O	1:A:62:VAL:HB	2.18	0.42
1:C:106:GLN:N	1:C:106:GLN:CD	2.73	0.42
1:C:92:TYR:O	1:C:97:LYS:HG2	2.19	0.42
2:D:395:VAL:C	2:D:397:LYS:N	2.72	0.42
1:A:120:PHE:CD1	1:A:154:LYS:HG2	2.54	0.42
1:A:62:VAL:HG13	1:A:67:TYR:CE2	2.55	0.42
1:C:124:GLN:O	1:C:128:GLU:HB2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:NZ	3:C:253:HOH:O	2.53	0.42
1:A:112:HIS:HB3	1:A:146:ARG:HD2	2.02	0.42
1:A:16:PHE:O	1:A:17:LYS:C	2.58	0.42
1:C:188:ASP:O	1:C:191:VAL:HG22	2.20	0.42
2:D:367:ASP:OD2	2:D:370:SER:HB2	2.19	0.42
1:A:146:ARG:HH22	2:B:370:SER:CB	2.27	0.42
1:A:197:TYR:O	1:A:198:GLY:C	2.58	0.42
1:C:100:LEU:HD11	1:C:129:ASN:HB2	2.02	0.42
1:C:37:ARG:HA	1:C:41:HIS:CD2	2.55	0.42
1:C:56:LEU:CB	3:C:232:HOH:O	2.64	0.42
1:A:74:THR:O	1:A:77:HIS:HB2	2.20	0.42
1:C:33:ASP:HB2	1:C:34:GLN:OE1	2.20	0.42
1:C:44:VAL:HG13	1:C:87:VAL:CG1	2.45	0.42
1:A:153:LEU:N	1:A:153:LEU:HD22	2.20	0.42
1:A:175:TRP:HH2	3:B:433:HOH:O	2.03	0.42
1:A:11:MET:HG2	1:A:46:PHE:HE2	1.85	0.42
1:A:94:ARG:HH11	1:A:94:ARG:HB2	1.84	0.42
1:C:135:ILE:H	1:C:135:ILE:CD1	2.33	0.41
1:C:15:PHE:C	1:C:15:PHE:CD2	2.93	0.41
2:D:348:GLU:HA	2:D:376:ASP:HA	2.01	0.41
1:A:176:THR:HB	3:A:285:HOH:O	2.19	0.41
1:C:112:HIS:CE1	3:C:268:HOH:O	2.74	0.41
1:A:174:GLY:O	1:A:205:ASP:HA	2.20	0.41
2:B:385:ALA:HB1	2:B:414:GLN:CD	2.41	0.41
1:C:154:LYS:HB2	1:C:154:LYS:HE3	1.83	0.41
1:C:59:MET:O	1:C:61:ASN:N	2.53	0.41
1:A:89:LYS:HG2	1:A:125:PHE:CE1	2.56	0.41
1:C:152:SER:HB3	1:C:155:LEU:HB2	2.01	0.41
1:C:178:LEU:HD12	1:C:193:LEU:HD12	2.02	0.41
1:A:94:ARG:NH1	1:A:94:ARG:HB2	2.36	0.41
1:A:73:TRP:HZ2	2:B:404:GLN:HG3	1.79	0.41
1:A:105:ASN:O	1:A:138:LYS:HE3	2.21	0.41
1:A:29:LEU:HD11	1:A:59:MET:HE3	2.02	0.41
2:B:380:GLY:HA2	2:B:383:ILE:HG12	2.02	0.41
1:A:150:VAL:HG23	1:A:151:GLY:N	2.35	0.41
1:A:38:ILE:O	1:A:41:HIS:HB2	2.20	0.41
1:A:52:THR:O	1:A:53:SER:C	2.59	0.41
1:A:33:ASP:OD1	1:A:33:ASP:C	2.59	0.41
1:C:166:ALA:HB1	1:C:169:TRP:CE2	2.56	0.41
1:A:178:LEU:HD13	1:A:193:LEU:HD12	2.03	0.41
1:C:14:GLU:OE2	3:C:239:HOH:O	2.22	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD23	1:C:39:PRO:HG2	2.02	0.41
1:C:225:LEU:N	1:C:225:LEU:CD1	2.84	0.41
2:D:349:ARG:HD2	2:D:351:LEU:HB2	2.02	0.41
1:C:152:SER:O	1:C:156:ILE:HG12	2.21	0.40
1:C:34:GLN:OE1	1:C:34:GLN:N	2.53	0.40
2:D:348:GLU:O	2:D:349:ARG:C	2.59	0.40
2:D:349:ARG:HD3	2:D:351:LEU:H	1.86	0.40
2:D:371:LEU:CD2	2:D:411:TYR:HB2	2.50	0.40
1:C:15:PHE:C	1:C:15:PHE:HD2	2.25	0.40
1:C:69:ASP:CG	1:C:73:TRP:HB2	2.41	0.40
1:A:120:PHE:CE1	1:A:154:LYS:HG2	2.57	0.40
1:A:172:LYS:C	1:A:174:GLY:N	2.74	0.40
1:A:204:VAL:HG12	3:A:238:HOH:O	2.21	0.40
1:A:39:PRO:O	1:A:40:LEU:C	2.59	0.40
1:C:178:LEU:O	1:C:179:PHE:C	2.59	0.40
2:D:371:LEU:HD22	2:D:411:TYR:CB	2.51	0.40
1:A:96:LEU:N	1:A:96:LEU:HD12	2.37	0.40
1:C:225:LEU:HA	1:C:228:VAL:CG2	2.51	0.40
1:C:157:GLU:OE2	1:C:192:LEU:HD21	2.21	0.40
2:D:348:GLU:N	2:D:377:SER:N	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:268:HOH:O	3:B:431:HOH:O[2_665]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	226/228 (99%)	170 (75%)	39 (17%)	17 (8%)	<b>1</b> <b>5</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	225/228 (99%)	173 (77%)	43 (19%)	9 (4%)	3	17
2	B	55/82 (67%)	43 (78%)	7 (13%)	5 (9%)	1	3
2	D	65/82 (79%)	45 (69%)	12 (18%)	8 (12%)	0	1
All	All	571/620 (92%)	431 (76%)	101 (18%)	39 (7%)	1	6

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	138	LYS
1	A	227	ASN
2	B	376	ASP
1	C	17	LYS
1	C	198	GLY
2	D	353	PHE
2	D	376	ASP
1	A	131	ALA
1	A	171	ASP
1	A	187	GLY
1	A	198	GLY
2	B	412	ALA
1	C	34	GLN
1	C	60	GLU
1	C	100	LEU
2	D	352	ILE
2	D	373	ILE
1	A	105	ASN
2	B	377	SER
2	B	414	GLN
2	B	415	VAL
1	C	13	ASN
1	C	208	GLY
2	D	351	LEU
2	D	366	ALA
1	A	34	GLN
1	A	52	THR
1	A	70	ASP
1	A	193	LEU
1	A	207	LYS
1	C	25	LYS
2	D	370	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	377	SER
1	A	161	GLY
1	A	164	LYS
1	A	95	PRO
1	A	220	VAL
1	C	161	GLY

### 5.3.2 Protein sidechains ⓘ

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	198/198 (100%)	184 (93%)	14 (7%)	14	46
1	C	197/198 (100%)	188 (95%)	9 (5%)	27	64
2	B	46/69 (67%)	38 (83%)	8 (17%)	2	10
2	D	54/69 (78%)	42 (78%)	12 (22%)	1	4
All	All	495/534 (93%)	452 (91%)	43 (9%)	10	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	GLN
1	A	17	LYS
1	A	74	THR
1	A	84	ASN
1	A	93	ASP
1	A	106	GLN
1	A	111	LEU
1	A	125	PHE
1	A	133	VAL
1	A	153	LEU
1	A	217	ASN
1	A	219	GLN
1	A	227	ASN
2	B	360	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	369	ASP
2	B	371	LEU
2	B	376	ASP
2	B	383	ILE
2	B	400	TYR
2	B	401	VAL
2	B	405	SER
1	C	15	PHE
1	C	19	GLN
1	C	20	GLU
1	C	23	HIS
1	C	49	HIS
1	C	61	ASN
1	C	84	ASN
1	C	128	GLU
1	C	217	ASN
2	D	349	ARG
2	D	351	LEU
2	D	353	PHE
2	D	361	SER
2	D	365	GLU
2	D	377	SER
2	D	388	GLN
2	D	396	ARG
2	D	400	TYR
2	D	404	GLN
2	D	405	SER
2	D	414	GLN

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

Mol	Chain	Res	Type
1	A	3	ASN
1	A	19	GLN
1	A	41	HIS
1	A	77	HIS
1	A	84	ASN
1	A	106	GLN
1	A	129	ASN
1	A	140	ASN
1	A	141	GLN
1	A	168	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	170	GLN
1	A	173	GLN
1	A	206	ASN
1	A	217	ASN
2	B	404	GLN
2	B	414	GLN
1	C	8	GLN
1	C	19	GLN
1	C	41	HIS
1	C	47	GLN
1	C	61	ASN
1	C	77	HIS
1	C	84	ASN
1	C	106	GLN
1	C	140	ASN
1	C	168	ASN
1	C	206	ASN
1	C	217	ASN
1	C	226	ASN
2	D	404	GLN

### 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.