



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:13 AM UTC

PDB ID : 1CA9 / pdb\_00001ca9  
Title : STRUCTURE OF TNF RECEPTOR ASSOCIATED FACTOR 2 IN COMPLEX WITH A PEPTIDE FROM TNF-R2  
Authors : Park, Y.C.; Burkitt, V.; Villa, A.R.; Tong, L.; Wu, H.  
Deposited on : 1999-02-25  
Resolution : 2.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

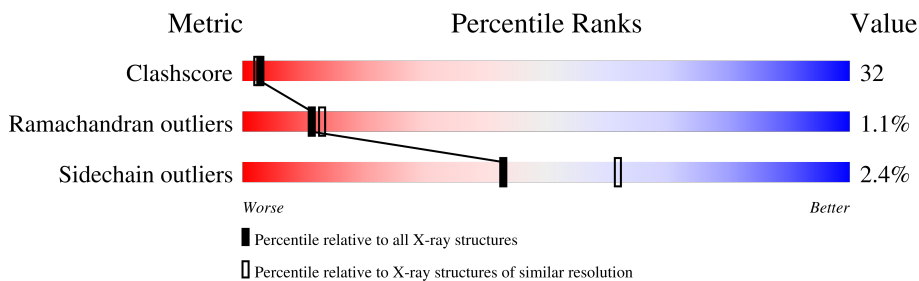
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	192	60% 36% ..
1	B	192	68% 31% ..
1	C	192	69% 28% ..
1	D	192	47% 45% 5% .
1	E	192	44% 49% ...
1	F	192	61% 31% ...
2	G	10	10% 50% 10% 30%
2	H	10	70% 20% 10%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9554 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 (TNF RECEPTOR ASSOCIATED FACTOR 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	Total 1435	C 919	N 242	O 264	S 10	0	0	0
1	B	191	Total 1417	C 904	N 241	O 262	S 10	0	0	0
1	C	191	Total 1440	C 921	N 243	O 266	S 10	0	0	0
1	D	186	Total 1406	C 901	N 241	O 254	S 10	0	0	0
1	E	186	Total 1410	C 902	N 240	O 258	S 10	0	0	0
1	F	186	Total 1401	C 895	N 238	O 258	S 10	0	0	0

- Molecule 2 is a protein called PROTEIN (TNF-R2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	7	Total 58	C 36	N 8	O 13	S 1	0	0	0
2	H	10	Total 77	C 48	N 11	O 17	S 1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	128	Total 128	O 128	0	0
3	B	140	Total 140	O 140	0	0
3	C	181	Total 181	O 181	0	0
3	D	134	Total 134	O 134	0	0

*Continued on next page...*

*Continued from previous page...*

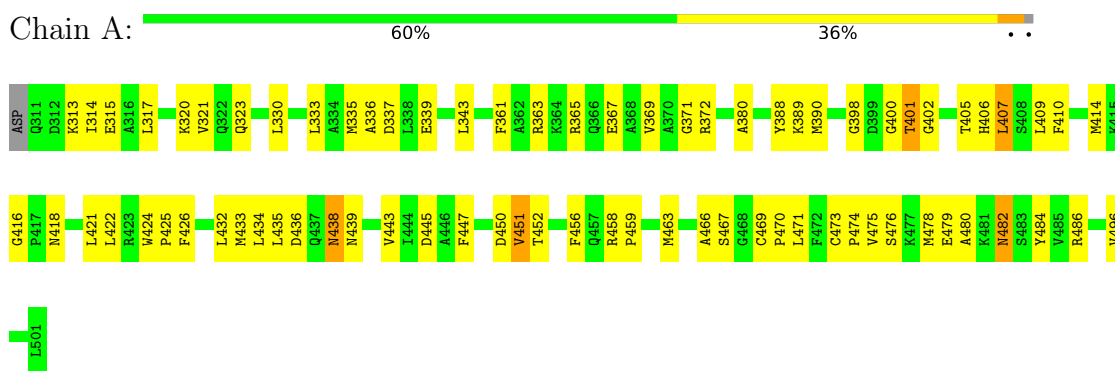
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	139	Total 139	O 139	0	0
3	F	159	Total 159	O 159	0	0
3	G	13	Total 13	O 13	0	0
3	H	16	Total 16	O 16	0	0

### 3 Residue-property plots i

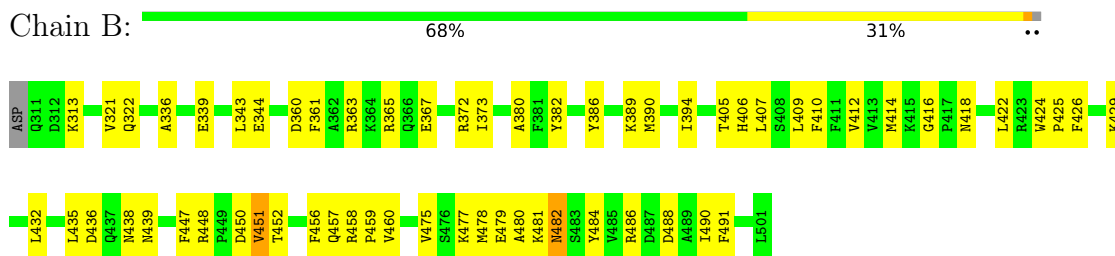
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

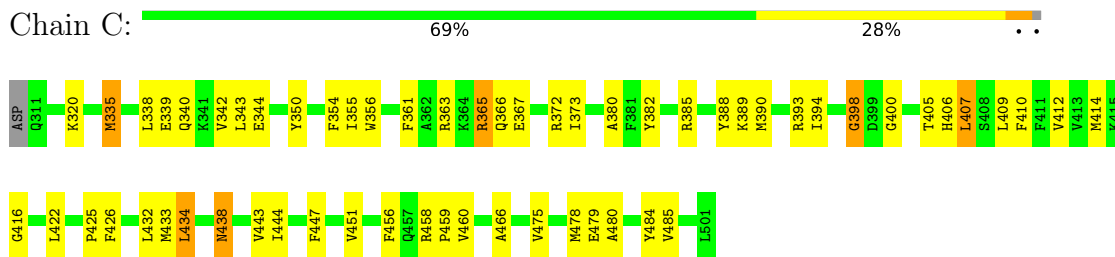
- Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)



- Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

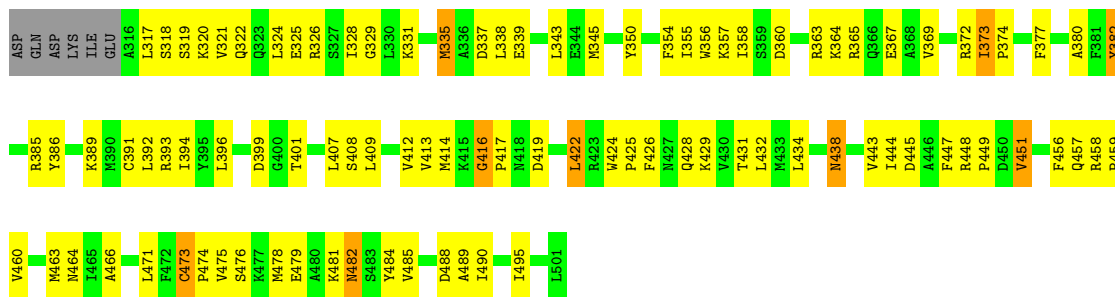


- Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

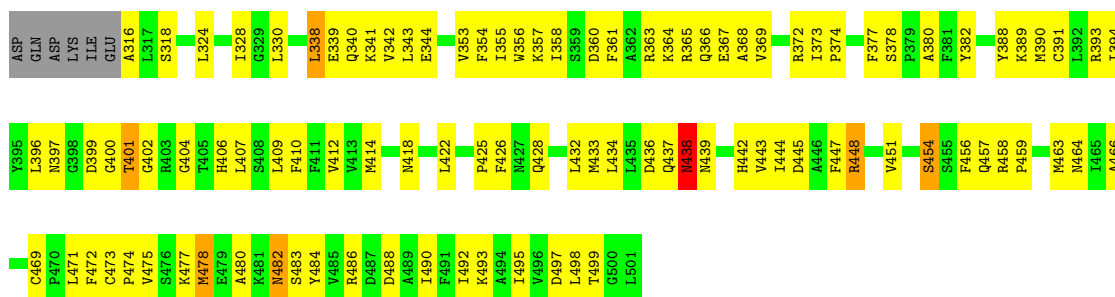


- Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

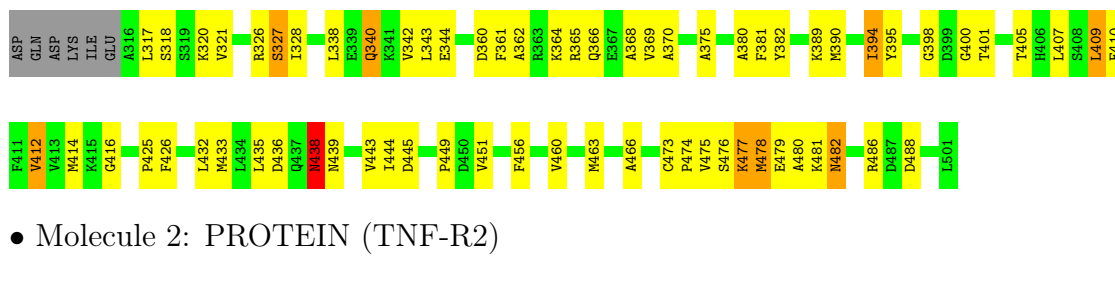




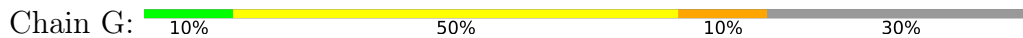
• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)



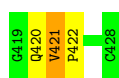
• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)



• Molecule 2: PROTEIN (TNF-R2)



• Molecule 2: PROTEIN (TNF-R2)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.00Å 84.40Å 100.70Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.2 (20.00-2.30)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.234 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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	0.47	0/1465	1.02	3/1987 (0.2%)
1	B	0.47	0/1447	1.03	9/1965 (0.5%)
1	C	0.48	0/1470	1.06	8/1993 (0.4%)
1	D	0.45	0/1436	1.06	12/1946 (0.6%)
1	E	0.46	0/1440	1.01	4/1951 (0.2%)
1	F	0.47	0/1431	1.05	8/1940 (0.4%)
2	G	0.42	0/59	0.93	0/75
2	H	0.65	0/78	1.63	2/102 (2.0%)
All	All	0.47	0/8826	1.04	46/11959 (0.4%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	VAL	N-CA-C	-12.13	100.83	112.96
1	C	460	VAL	N-CA-C	-8.77	104.27	111.81
2	H	421	VAL	CA-C-N	-8.76	110.37	119.83
2	H	421	VAL	C-N-CA	-8.76	110.37	119.83
1	F	398	GLY	N-CA-C	8.25	123.37	112.65
1	F	460	VAL	N-CA-C	-7.91	105.05	112.96
1	D	328	ILE	N-CA-C	-7.78	102.49	113.07
1	C	373	ILE	CA-C-N	7.70	126.98	118.97
1	C	373	ILE	C-N-CA	7.70	126.98	118.97
1	D	460	VAL	N-CA-C	-7.48	105.48	112.96
1	D	438	ASN	N-CA-C	-6.92	104.72	113.72
1	A	398	GLY	N-CA-C	6.62	121.01	112.68
1	F	438	ASN	N-CA-C	-6.43	103.96	113.61
1	C	438	ASN	N-CA-C	-6.37	105.43	113.72
1	A	435	LEU	N-CA-C	6.31	119.80	109.76
1	D	416	GLY	CA-C-N	6.22	125.90	119.56
1	D	416	GLY	C-N-CA	6.22	125.90	119.56
1	C	434	LEU	N-CA-C	-6.03	97.32	107.99
1	E	448	ARG	CA-C-N	6.01	126.95	119.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	448	ARG	C-N-CA	6.01	126.95	119.98
1	E	438	ASN	N-CA-C	-6.01	104.07	113.02
1	F	435	LEU	N-CA-C	6.00	118.70	110.24
1	B	416	GLY	CA-C-N	5.83	125.51	119.56
1	B	416	GLY	C-N-CA	5.83	125.51	119.56
1	B	382	TYR	N-CA-C	5.57	118.15	109.52
1	C	398	GLY	N-CA-C	5.55	119.87	112.65
1	B	412	VAL	N-CA-C	5.52	116.01	107.78
1	C	416	GLY	CA-C-N	5.48	125.19	119.82
1	C	416	GLY	C-N-CA	5.48	125.19	119.82
1	B	435	LEU	N-CA-C	5.42	118.30	110.28
1	F	412	VAL	N-CA-C	5.39	115.75	107.77
1	B	336	ALA	N-CA-C	-5.38	104.82	111.33
1	F	416	GLY	CA-C-N	5.34	124.96	119.56
1	F	416	GLY	C-N-CA	5.34	124.96	119.56
1	D	382	TYR	N-CA-C	5.33	117.96	109.81
1	B	373	ILE	CA-C-N	5.28	124.46	118.97
1	B	373	ILE	C-N-CA	5.28	124.46	118.97
1	A	407	LEU	N-CA-C	-5.21	101.28	109.25
1	E	454	SER	N-CA-C	-5.18	107.01	113.38
1	F	394	ILE	N-CA-C	5.13	116.11	108.46
1	D	458	ARG	CA-C-N	5.06	125.06	119.90
1	D	458	ARG	C-N-CA	5.06	125.06	119.90
1	D	373	ILE	CA-C-N	5.06	124.36	118.85
1	D	373	ILE	C-N-CA	5.06	124.36	118.85
1	D	473	CYS	CA-C-N	5.02	125.25	119.83
1	D	473	CYS	C-N-CA	5.02	125.25	119.83

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	1435	0	1375	78	0
1	B	1417	0	1322	67	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1440	0	1375	54	0
1	D	1406	0	1354	114	0
1	E	1410	0	1357	161	0
1	F	1401	0	1331	70	0
2	G	58	0	51	16	0
2	H	77	0	68	15	0
3	A	128	0	0	20	0
3	B	140	0	0	16	0
3	C	181	0	0	12	0
3	D	134	0	0	50	0
3	E	139	0	0	80	0
3	F	159	0	0	17	0
3	G	13	0	0	0	0
3	H	16	0	0	3	0
All	All	9554	0	8233	543	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 32.

All (543) 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:448:ARG:HB2	2:H:421:VAL:CG1	1.73	1.17
1:B:448:ARG:HB2	2:H:421:VAL:HG13	1.11	1.11
1:B:448:ARG:HD2	2:H:421:VAL:HG22	1.41	1.02
1:C:338:LEU:HG	3:C:6769:HOH:O	1.60	1.01
1:C:389:LYS:HG2	1:C:414:MET:HE3	1.40	1.01
1:B:448:ARG:HD2	2:H:421:VAL:CG2	1.91	0.99
1:D:422:LEU:HB2	3:D:6860:HOH:O	1.64	0.98
1:E:426:PHE:HA	3:E:6858:HOH:O	1.61	0.97
1:E:389:LYS:HG2	1:E:414:MET:HE3	1.42	0.97
1:E:373:ILE:HD12	2:G:425:LYS:NZ	1.80	0.97
2:H:420:GLN:HG2	2:H:421:VAL:HG23	1.45	0.96
1:E:355:ILE:HA	3:E:6537:HOH:O	1.65	0.96
1:B:448:ARG:CB	2:H:421:VAL:HG13	1.95	0.95
1:F:389:LYS:HG2	1:F:414:MET:HE3	1.46	0.95
1:E:477:LYS:HD2	3:E:6596:HOH:O	1.68	0.93
1:F:409:LEU:HD22	1:F:432:LEU:HD13	1.48	0.93
1:D:425:PRO:HG3	1:D:451:VAL:HG13	1.50	0.90
1:F:409:LEU:HG	3:F:6761:HOH:O	1.72	0.90
1:D:489:ALA:HB1	3:D:6739:HOH:O	1.70	0.90

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:HG2	1:B:414:MET:HE3	1.51	0.89
1:C:433:MET:HE2	1:C:444:ILE:HD12	1.53	0.89
1:D:459:PRO:HG3	1:D:464:ASN:HD21	1.37	0.89
1:A:409:LEU:HG	3:A:6158:HOH:O	1.71	0.89
1:A:409:LEU:HD22	1:A:432:LEU:HD13	1.56	0.86
1:A:317:LEU:HD21	3:B:6849:HOH:O	1.74	0.86
1:E:367:GLU:HB3	3:E:6825:HOH:O	1.73	0.86
1:E:474:PRO:HG3	3:E:6767:HOH:O	1.75	0.86
1:A:380:ALA:CB	1:A:414:MET:HE1	2.05	0.85
1:C:380:ALA:HB2	1:C:414:MET:HE1	1.56	0.85
1:B:380:ALA:CB	1:B:414:MET:HE1	2.07	0.85
1:C:335:MET:HA	1:C:335:MET:HE3	1.59	0.84
1:D:393:ARG:HG3	3:D:6861:HOH:O	1.77	0.83
1:A:389:LYS:HG2	1:A:414:MET:HE3	1.59	0.83
1:E:396:LEU:HA	3:E:6298:HOH:O	1.77	0.83
1:C:366:GLN:HG3	3:C:6536:HOH:O	1.79	0.83
1:E:358:ILE:HD11	3:E:6403:HOH:O	1.76	0.83
1:A:425:PRO:HG3	1:A:451:VAL:HG13	1.61	0.82
1:E:355:ILE:HG12	3:E:6537:HOH:O	1.78	0.82
1:B:380:ALA:HB2	1:B:414:MET:HE1	1.59	0.82
1:C:339:GLU:O	1:C:343:LEU:HD13	1.80	0.81
1:E:482:ASN:HB3	3:E:6023:HOH:O	1.78	0.81
1:E:493:LYS:HA	3:E:6537:HOH:O	1.79	0.81
1:E:373:ILE:HD12	2:G:425:LYS:HZ2	1.44	0.81
1:C:380:ALA:CB	1:C:414:MET:HE1	2.11	0.81
1:E:457:GLN:HG2	3:E:6137:HOH:O	1.79	0.81
1:E:369:VAL:HA	3:E:6870:HOH:O	1.81	0.80
1:E:409:LEU:HD22	1:E:432:LEU:HD13	1.63	0.80
1:B:448:ARG:CD	2:H:421:VAL:HG22	2.11	0.79
1:A:482:ASN:HD22	1:A:482:ASN:H	1.30	0.79
1:E:407:LEU:HG	3:E:6298:HOH:O	1.83	0.78
1:E:493:LYS:HG3	3:E:6537:HOH:O	1.82	0.78
1:D:414:MET:HG3	3:D:6465:HOH:O	1.81	0.78
1:C:363:ARG:HD3	3:C:6300:HOH:O	1.84	0.77
1:D:482:ASN:HD22	1:D:482:ASN:H	1.33	0.76
1:A:407:LEU:HD12	3:A:6619:HOH:O	1.84	0.76
1:D:495:ILE:HB	3:D:6759:HOH:O	1.85	0.76
1:A:380:ALA:HB2	1:A:414:MET:HE1	1.66	0.76
1:D:389:LYS:HG2	1:D:414:MET:HE3	1.67	0.76
1:E:493:LYS:HG2	3:E:6446:HOH:O	1.86	0.76
1:D:459:PRO:HG3	1:D:464:ASN:ND2	2.00	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:420:GLN:CG	2:H:421:VAL:HG23	2.16	0.76
1:D:377:PHE:HA	3:D:6861:HOH:O	1.86	0.75
1:B:425:PRO:HG3	1:B:451:VAL:HG13	1.68	0.75
1:C:394:ILE:HD11	1:C:407:LEU:HD21	1.68	0.75
1:E:393:ARG:HG3	3:E:6779:HOH:O	1.85	0.75
1:C:425:PRO:HG3	1:C:451:VAL:HG13	1.69	0.75
1:E:401:THR:O	1:E:471:LEU:HD21	1.87	0.75
1:B:409:LEU:HD22	1:B:432:LEU:HD13	1.68	0.74
1:D:425:PRO:CG	1:D:451:VAL:HG13	2.17	0.74
1:D:372:ARG:HD3	3:D:6290:HOH:O	1.87	0.74
1:F:380:ALA:CB	1:F:414:MET:HE1	2.17	0.74
1:D:380:ALA:HB2	1:D:414:MET:HE1	1.67	0.74
1:B:361:PHE:O	1:B:365:ARG:HB2	1.88	0.73
1:D:475:VAL:HG11	3:D:6652:HOH:O	1.89	0.73
1:C:390:MET:C	1:C:414:MET:HE2	2.13	0.73
1:D:482:ASN:HD22	1:D:482:ASN:N	1.86	0.73
1:F:340:GLN:O	1:F:344:GLU:HG3	1.90	0.72
1:B:482:ASN:H	1:B:482:ASN:HD22	1.35	0.72
1:A:445:ASP:HB2	3:A:6258:HOH:O	1.89	0.72
1:E:442:HIS:HB3	3:E:6401:HOH:O	1.89	0.72
1:F:394:ILE:HD11	1:F:407:LEU:HD21	1.72	0.72
1:A:315:GLU:HG2	3:A:6356:HOH:O	1.90	0.71
1:D:409:LEU:HD22	1:D:432:LEU:HD13	1.72	0.71
1:D:331:LYS:HZ1	1:E:328:ILE:HG22	1.54	0.71
1:D:396:LEU:HB2	3:D:6760:HOH:O	1.91	0.71
1:E:372:ARG:CD	2:G:423:PHE:HB2	2.21	0.71
1:E:402:GLY:HA2	3:E:6589:HOH:O	1.89	0.70
1:C:409:LEU:HD22	1:C:432:LEU:HD13	1.73	0.70
1:B:448:ARG:HD3	3:B:6270:HOH:O	1.90	0.70
1:E:377:PHE:HA	3:E:6779:HOH:O	1.92	0.70
1:E:459:PRO:HG3	1:E:464:ASN:ND2	2.07	0.70
1:D:386:TYR:HE2	3:E:6410:HOH:O	1.74	0.69
1:D:485:VAL:HG13	3:D:6809:HOH:O	1.93	0.68
1:F:362:ALA:HB3	3:F:6889:HOH:O	1.94	0.68
1:B:448:ARG:HD2	2:H:421:VAL:HG21	1.73	0.68
1:E:442:HIS:HB2	3:E:6217:HOH:O	1.93	0.68
1:F:326:ARG:HA	3:F:6612:HOH:O	1.93	0.68
1:B:438:ASN:HB2	3:B:6584:HOH:O	1.94	0.67
1:E:339:GLU:O	1:E:343:LEU:HD13	1.95	0.67
1:E:373:ILE:HD12	2:G:425:LYS:HZ1	1.58	0.67
1:F:481:LYS:HE2	3:F:6888:HOH:O	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ALA:HB1	1:A:414:MET:HE1	1.77	0.67
1:E:380:ALA:HB2	1:E:414:MET:HE1	1.77	0.67
1:F:368:ALA:HB1	3:F:6533:HOH:O	1.94	0.67
1:F:482:ASN:HD22	1:F:482:ASN:H	1.41	0.67
1:E:459:PRO:HG3	1:E:464:ASN:HD21	1.60	0.67
1:B:448:ARG:HB2	2:H:421:VAL:HG11	1.72	0.66
1:C:363:ARG:O	1:C:367:GLU:HG3	1.95	0.66
1:E:330:LEU:HD13	3:E:6368:HOH:O	1.95	0.66
2:H:421:VAL:HA	3:H:6186:HOH:O	1.94	0.66
1:D:365:ARG:HA	3:D:6760:HOH:O	1.95	0.66
1:E:356:TRP:HZ3	3:E:6780:HOH:O	1.78	0.66
1:E:365:ARG:HB3	3:E:6824:HOH:O	1.95	0.66
1:E:444:ILE:HB	3:E:6217:HOH:O	1.95	0.66
1:F:425:PRO:HG3	1:F:451:VAL:HG13	1.76	0.66
1:F:327:SER:HA	3:F:6590:HOH:O	1.95	0.66
1:D:331:LYS:NZ	1:E:328:ILE:HG22	2.10	0.66
1:B:313:LYS:HA	3:B:6848:HOH:O	1.95	0.66
1:F:380:ALA:HB2	1:F:414:MET:HE1	1.78	0.65
1:E:388:TYR:CE1	3:E:6858:HOH:O	2.48	0.65
1:E:434:LEU:HG	1:E:484:TYR:HD2	1.60	0.65
1:E:363:ARG:O	1:E:367:GLU:HG3	1.96	0.64
1:D:380:ALA:CB	1:D:414:MET:HE1	2.28	0.63
1:E:353:VAL:HG12	3:E:6410:HOH:O	1.98	0.63
1:D:363:ARG:O	1:D:367:GLU:HG3	1.98	0.63
1:E:361:PHE:HB3	3:E:6388:HOH:O	1.98	0.63
1:E:400:GLY:C	1:E:402:GLY:H	2.07	0.63
1:F:390:MET:C	1:F:414:MET:HE2	2.24	0.62
1:E:409:LEU:HD11	3:E:6464:HOH:O	1.99	0.62
1:B:322:GLN:HA	3:B:6538:HOH:O	1.98	0.62
1:D:335:MET:HE3	1:D:335:MET:HA	1.82	0.62
1:F:389:LYS:HG2	1:F:414:MET:CE	2.26	0.62
1:B:365:ARG:NH2	1:B:475:VAL:CG1	2.63	0.62
1:D:431:THR:HB	3:D:6759:HOH:O	2.00	0.61
1:D:374:PRO:HD2	3:D:6066:HOH:O	1.98	0.61
1:B:482:ASN:HD22	1:B:482:ASN:N	1.94	0.61
1:D:481:LYS:HG3	3:D:6476:HOH:O	1.99	0.61
1:A:390:MET:C	1:A:414:MET:HE2	2.26	0.61
1:F:370:ALA:HA	3:F:6127:HOH:O	2.00	0.61
1:D:325:GLU:O	1:D:326:ARG:HD3	1.99	0.60
1:D:393:ARG:HA	3:D:6861:HOH:O	2.02	0.60
1:E:406:HIS:CE1	1:E:471:LEU:HD22	2.36	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:GLU:O	1:D:343:LEU:HD13	2.01	0.60
1:E:397:ASN:ND2	3:E:6870:HOH:O	2.34	0.60
1:A:361:PHE:O	1:A:365:ARG:HB2	2.01	0.60
1:E:388:TYR:CD1	1:E:422:LEU:HD23	2.37	0.60
1:E:498:LEU:HD22	3:E:6508:HOH:O	2.01	0.60
1:E:374:PRO:HA	3:E:6510:HOH:O	2.02	0.59
1:F:365:ARG:NH2	1:F:475:VAL:HG13	2.17	0.59
1:D:357:LYS:HG2	3:D:6739:HOH:O	2.03	0.59
1:E:380:ALA:CB	1:E:414:MET:HE1	2.32	0.59
1:C:372:ARG:HG3	3:C:6103:HOH:O	2.03	0.59
1:A:482:ASN:HD22	1:A:482:ASN:N	1.94	0.58
1:E:324:LEU:HA	3:E:6540:HOH:O	2.03	0.58
1:E:389:LYS:HG2	1:E:414:MET:CE	2.28	0.58
1:F:380:ALA:HB1	1:F:414:MET:HE1	1.85	0.58
1:B:390:MET:C	1:B:414:MET:HE2	2.29	0.58
1:F:318:SER:C	3:F:6455:HOH:O	2.47	0.58
1:D:363:ARG:HD3	3:D:6051:HOH:O	2.03	0.57
1:E:358:ILE:HG13	3:E:6426:HOH:O	2.03	0.57
1:B:448:ARG:HG3	3:H:6186:HOH:O	2.03	0.57
1:D:426:PHE:CZ	1:D:428:GLN:HB2	2.39	0.57
1:E:360:ASP:HA	1:E:488:ASP:OD2	2.05	0.57
1:B:380:ALA:HB1	1:B:414:MET:HE1	1.85	0.57
1:E:367:GLU:CD	2:G:425:LYS:HZ3	2.12	0.57
1:B:409:LEU:HB3	3:B:6399:HOH:O	2.03	0.57
1:E:365:ARG:NH2	1:E:475:VAL:CG1	2.67	0.57
1:D:414:MET:HG2	1:D:463:MET:HG2	1.86	0.57
1:E:482:ASN:H	1:E:482:ASN:HD22	1.51	0.57
1:E:357:LYS:C	3:E:6426:HOH:O	2.48	0.56
1:E:356:TRP:CD1	3:E:6426:HOH:O	2.58	0.56
1:E:436:ASP:C	1:E:438:ASN:H	2.13	0.56
1:F:365:ARG:O	1:F:365:ARG:HD3	2.03	0.56
1:B:365:ARG:NH2	1:B:475:VAL:HG13	2.20	0.56
1:C:340:GLN:O	1:C:344:GLU:HG3	2.05	0.56
1:D:350:TYR:CD2	1:D:385:ARG:HA	2.41	0.56
1:E:412:VAL:HG22	1:E:466:ALA:HB2	1.88	0.56
1:C:434:LEU:HB3	1:C:443:VAL:HB	1.88	0.56
1:E:433:MET:HB3	3:E:6401:HOH:O	2.05	0.56
1:D:338:LEU:HD22	1:F:338:LEU:HD21	1.88	0.56
1:D:365:ARG:HH11	1:D:369:VAL:CG2	2.19	0.56
1:A:389:LYS:C	1:A:390:MET:HG3	2.31	0.55
1:B:425:PRO:CG	1:B:451:VAL:HG13	2.36	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:PHE:HD2	3:D:6677:HOH:O	1.89	0.55
1:F:476:SER:C	1:F:478:MET:H	2.13	0.55
1:E:406:HIS:ND1	1:E:471:LEU:HD22	2.22	0.55
1:E:457:GLN:N	3:E:6137:HOH:O	2.39	0.55
1:D:322:GLN:O	1:D:326:ARG:HG2	2.07	0.55
1:F:361:PHE:O	1:F:365:ARG:HB2	2.06	0.55
1:D:425:PRO:HG3	1:D:451:VAL:CG1	2.32	0.55
1:D:448:ARG:HG2	1:D:448:ARG:HH11	1.72	0.55
1:E:367:GLU:CD	2:G:425:LYS:NZ	2.65	0.55
1:A:426:PHE:HZ	3:A:6369:HOH:O	1.88	0.54
1:D:391:CYS:N	3:D:6465:HOH:O	2.40	0.54
1:E:354:PHE:CE2	1:E:356:TRP:HB2	2.42	0.54
1:E:492:ILE:HG13	3:E:6768:HOH:O	2.07	0.54
1:F:365:ARG:HH11	1:F:369:VAL:CG2	2.20	0.54
1:B:409:LEU:HD23	1:B:410:PHE:N	2.22	0.54
1:E:372:ARG:HB2	3:E:6825:HOH:O	2.06	0.54
1:E:373:ILE:HG13	3:E:6825:HOH:O	2.07	0.54
1:F:409:LEU:HD23	1:F:410:PHE:N	2.22	0.54
1:C:388:TYR:CD2	1:C:422:LEU:HD23	2.43	0.54
1:F:320:LYS:HA	3:F:6900:HOH:O	2.08	0.54
1:A:436:ASP:C	1:A:438:ASN:H	2.15	0.54
1:D:417:PRO:HA	3:E:6835:HOH:O	2.07	0.54
1:F:321:VAL:C	3:F:6845:HOH:O	2.51	0.54
1:E:426:PHE:HB3	1:E:456:PHE:HB3	1.89	0.54
1:E:469:CYS:HB3	3:E:6122:HOH:O	2.07	0.54
2:H:421:VAL:HG12	2:H:421:VAL:O	2.08	0.54
1:E:358:ILE:CG1	3:E:6426:HOH:O	2.56	0.54
1:E:495:ILE:HG13	3:E:6446:HOH:O	2.07	0.54
1:E:456:PHE:N	3:E:6137:HOH:O	2.40	0.54
1:F:365:ARG:NH2	1:F:475:VAL:CG1	2.71	0.53
1:E:409:LEU:HD23	1:E:410:PHE:N	2.23	0.53
1:E:367:GLU:OE2	2:G:425:LYS:HE2	2.08	0.53
1:C:425:PRO:CG	1:C:451:VAL:HG13	2.38	0.53
1:E:498:LEU:HB3	3:E:6508:HOH:O	2.09	0.53
1:A:450:ASP:O	1:A:452:THR:N	2.41	0.53
1:B:481:LYS:HA	3:B:6307:HOH:O	2.08	0.53
1:E:316:ALA:C	3:E:6646:HOH:O	2.51	0.53
1:A:480:ALA:HB2	3:A:6578:HOH:O	2.08	0.53
1:C:409:LEU:HD23	1:C:410:PHE:N	2.23	0.53
1:D:326:ARG:HA	3:D:6583:HOH:O	2.09	0.53
1:E:396:LEU:HD23	3:E:6298:HOH:O	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:VAL:HG22	1:F:477:LYS:HE2	1.90	0.53
1:B:436:ASP:C	1:B:438:ASN:H	2.16	0.53
1:D:476:SER:C	1:D:478:MET:H	2.17	0.53
1:E:363:ARG:HH22	1:E:364:LYS:HE2	1.74	0.53
1:F:409:LEU:CD2	1:F:432:LEU:HD13	2.31	0.53
1:A:425:PRO:CG	1:A:451:VAL:HG13	2.37	0.52
1:C:342:VAL:CG2	3:C:6769:HOH:O	2.57	0.52
1:F:405:THR:O	1:F:475:VAL:HG23	2.09	0.52
1:D:382:TYR:N	1:D:382:TYR:CD1	2.76	0.52
1:D:407:LEU:C	1:D:407:LEU:HD23	2.34	0.52
1:A:333:LEU:O	1:A:336:ALA:HB3	2.09	0.52
1:A:390:MET:SD	3:A:6369:HOH:O	2.59	0.52
1:C:434:LEU:HG	1:C:484:TYR:CD2	2.45	0.52
2:H:421:VAL:O	2:H:422:PRO:C	2.46	0.52
1:B:389:LYS:HG2	1:B:414:MET:CE	2.33	0.52
1:F:482:ASN:HD22	1:F:482:ASN:N	2.01	0.52
1:B:363:ARG:O	1:B:367:GLU:HG3	2.10	0.52
1:E:316:ALA:HB1	3:E:6864:HOH:O	2.09	0.52
1:C:372:ARG:HB3	3:C:6002:HOH:O	2.11	0.51
1:C:394:ILE:HD11	1:C:407:LEU:CD2	2.39	0.51
1:E:356:TRP:CD2	3:E:6403:HOH:O	2.62	0.51
1:F:340:GLN:OE1	1:F:340:GLN:HA	2.10	0.51
2:H:420:GLN:CD	2:H:421:VAL:HG23	2.34	0.51
1:C:447:PHE:CD1	1:C:447:PHE:C	2.89	0.51
1:D:389:LYS:HG2	1:D:414:MET:CE	2.39	0.51
1:D:449:PRO:HB3	1:D:456:PHE:CD2	2.45	0.51
1:D:490:ILE:HG23	3:D:6809:HOH:O	2.09	0.51
1:B:426:PHE:HB3	1:B:456:PHE:HB3	1.92	0.51
1:D:419:ASP:HA	3:D:6860:HOH:O	2.11	0.51
1:E:390:MET:C	1:E:414:MET:HE2	2.35	0.51
1:C:479:GLU:OE1	1:C:479:GLU:HA	2.10	0.51
1:A:439:ASN:HB2	3:A:6895:HOH:O	2.10	0.51
1:C:400:GLY:HA3	3:C:6635:HOH:O	2.11	0.51
1:E:418:ASN:O	1:E:422:LEU:HD13	2.10	0.51
1:E:358:ILE:CG1	3:E:6403:HOH:O	2.58	0.51
1:E:409:LEU:HD23	1:E:409:LEU:C	2.36	0.51
1:D:386:TYR:CE1	1:E:355:ILE:HB	2.46	0.50
1:E:434:LEU:HG	1:E:484:TYR:CD2	2.44	0.50
1:F:426:PHE:HB3	1:F:456:PHE:HB3	1.93	0.50
1:D:364:LYS:NZ	3:D:6164:HOH:O	2.43	0.50
1:E:406:HIS:CD2	3:E:6767:HOH:O	2.64	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:GLN:HG2	3:E:6824:HOH:O	2.11	0.50
1:E:434:LEU:N	3:E:6401:HOH:O	2.41	0.50
1:A:418:ASN:O	1:A:422:LEU:HD13	2.10	0.50
1:E:406:HIS:CE1	3:E:6767:HOH:O	2.64	0.50
1:C:426:PHE:HB3	1:C:456:PHE:HB3	1.93	0.50
1:D:360:ASP:O	1:D:364:LYS:HG3	2.12	0.50
1:F:478:MET:HA	1:F:482:ASN:OD1	2.12	0.50
1:F:360:ASP:HB2	1:F:364:LYS:HE3	1.94	0.50
1:E:400:GLY:O	1:E:402:GLY:N	2.44	0.50
1:E:324:LEU:O	1:E:328:ILE:HG13	2.11	0.50
1:E:477:LYS:HE3	3:E:6770:HOH:O	2.10	0.50
1:C:320:LYS:CB	3:C:6581:HOH:O	2.59	0.49
1:F:365:ARG:NH1	1:F:369:VAL:CG2	2.75	0.49
1:E:365:ARG:NH2	1:E:475:VAL:HG13	2.27	0.49
1:E:407:LEU:O	1:E:472:PHE:HB3	2.12	0.49
1:E:426:PHE:CZ	1:E:428:GLN:HB2	2.46	0.49
1:A:317:LEU:O	1:A:321:VAL:HG23	2.13	0.49
1:C:412:VAL:HG22	1:C:466:ALA:HB2	1.94	0.49
1:D:447:PHE:CD1	1:D:447:PHE:C	2.90	0.49
1:A:365:ARG:NH2	1:A:475:VAL:CG1	2.76	0.49
1:E:473:CYS:SG	1:E:477:LYS:HD3	2.53	0.49
1:A:466:ALA:HB3	2:G:427:GLU:OE2	2.12	0.49
1:D:385:ARG:NH1	3:D:6378:HOH:O	2.45	0.49
1:D:389:LYS:NZ	3:D:6539:HOH:O	2.45	0.49
1:E:443:VAL:HG23	1:E:484:TYR:CE2	2.48	0.49
1:C:478:MET:C	1:C:480:ALA:H	2.20	0.49
1:E:356:TRP:CE3	1:E:378:SER:HB3	2.48	0.49
1:E:425:PRO:HG3	1:E:451:VAL:HG13	1.95	0.49
1:D:479:GLU:HA	1:D:479:GLU:OE1	2.12	0.49
1:A:330:LEU:O	1:A:330:LEU:HD23	2.12	0.49
1:A:496:VAL:HG11	3:A:6369:HOH:O	2.12	0.49
1:A:365:ARG:NH2	1:A:475:VAL:HG13	2.28	0.48
1:D:373:ILE:HG23	3:D:6066:HOH:O	2.12	0.48
1:E:372:ARG:HD2	2:G:423:PHE:HB2	1.95	0.48
1:F:360:ASP:HA	1:F:488:ASP:OD2	2.14	0.48
1:D:338:LEU:O	1:D:338:LEU:HD23	2.13	0.48
1:D:412:VAL:HG22	1:D:466:ALA:HB2	1.94	0.48
1:E:478:MET:C	1:E:480:ALA:H	2.21	0.48
1:A:434:LEU:HB3	1:A:443:VAL:HB	1.95	0.48
1:D:392:LEU:C	3:D:6859:HOH:O	2.56	0.48
1:D:448:ARG:HG2	1:D:448:ARG:NH1	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:LYS:CG	1:E:414:MET:HE3	2.30	0.48
1:E:382:TYR:N	1:E:382:TYR:CD1	2.80	0.48
2:G:428:CYS:SG	2:G:428:CYS:O	2.71	0.48
1:B:429:LYS:HB2	1:B:448:ARG:NH1	2.29	0.48
1:D:457:GLN:HB3	3:D:6407:HOH:O	2.13	0.48
1:D:482:ASN:N	1:D:482:ASN:ND2	2.59	0.48
1:E:474:PRO:HG2	3:E:6596:HOH:O	2.14	0.48
1:A:405:THR:O	1:A:475:VAL:HG23	2.14	0.47
1:A:434:LEU:HG	1:A:484:TYR:HD2	1.79	0.47
1:F:473:CYS:SG	1:F:477:LYS:HD3	2.55	0.47
1:D:331:LYS:HD3	3:D:6789:HOH:O	2.13	0.47
1:B:447:PHE:CD1	1:B:447:PHE:C	2.91	0.47
1:D:317:LEU:O	1:D:318:SER:C	2.57	0.47
1:D:365:ARG:NH2	1:D:475:VAL:CG1	2.77	0.47
1:E:356:TRP:CZ3	1:E:378:SER:HB3	2.49	0.47
1:F:394:ILE:CD1	1:F:407:LEU:HD21	2.44	0.47
1:A:314:ILE:CB	3:A:6869:HOH:O	2.61	0.47
1:A:433:MET:SD	3:A:6773:HOH:O	2.61	0.47
1:A:447:PHE:C	1:A:447:PHE:CD1	2.91	0.47
1:D:326:ARG:CA	3:D:6583:HOH:O	2.62	0.47
1:D:394:ILE:HG13	1:D:408:SER:O	2.14	0.47
1:D:424:TRP:HH2	3:D:6799:HOH:O	1.96	0.47
1:A:414:MET:HG2	1:A:463:MET:HG2	1.97	0.47
1:D:429:LYS:HB2	1:D:448:ARG:NH1	2.29	0.47
1:E:482:ASN:HD22	1:E:482:ASN:N	2.08	0.47
1:F:463:MET:HG3	3:F:6379:HOH:O	2.14	0.47
1:B:360:ASP:HB3	3:B:6821:HOH:O	2.14	0.47
1:E:393:ARG:N	3:E:6793:HOH:O	2.48	0.47
1:E:397:ASN:O	1:E:404:GLY:N	2.46	0.47
1:E:400:GLY:C	1:E:402:GLY:N	2.70	0.47
1:F:433:MET:HE2	1:F:444:ILE:HD12	1.97	0.47
1:B:389:LYS:C	1:B:390:MET:HG3	2.39	0.47
1:D:416:GLY:H	1:D:419:ASP:CG	2.22	0.47
1:B:478:MET:HA	1:B:482:ASN:OD1	2.15	0.47
1:E:365:ARG:NH2	1:E:475:VAL:HG11	2.29	0.47
1:D:394:ILE:HD11	1:D:407:LEU:HD21	1.97	0.47
1:E:358:ILE:CD1	3:E:6403:HOH:O	2.48	0.47
1:E:454:SER:C	3:E:6137:HOH:O	2.56	0.47
1:F:365:ARG:NH1	1:F:369:VAL:HG22	2.30	0.47
1:D:365:ARG:HD2	3:D:6425:HOH:O	2.15	0.46
1:E:372:ARG:HD3	2:G:423:PHE:HB2	1.95	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:GLY:N	3:F:6557:HOH:O	2.43	0.46
1:A:434:LEU:HG	1:A:484:TYR:CD2	2.50	0.46
1:B:386:TYR:CE1	1:C:355:ILE:HB	2.51	0.46
1:C:335:MET:HA	1:C:335:MET:CE	2.37	0.46
1:D:399:ASP:HA	3:D:6724:HOH:O	2.16	0.46
1:D:431:THR:CB	3:D:6759:HOH:O	2.63	0.46
1:D:329:GLY:N	3:D:6583:HOH:O	2.46	0.46
1:E:361:PHE:O	1:E:365:ARG:HB2	2.15	0.46
1:D:426:PHE:HB3	1:D:456:PHE:HB3	1.97	0.46
1:A:363:ARG:O	1:A:367:GLU:HG3	2.16	0.46
1:D:365:ARG:NH2	1:D:475:VAL:HG13	2.31	0.46
1:E:444:ILE:HG12	1:E:445:ASP:N	2.30	0.46
1:D:473:CYS:HA	1:D:474:PRO:HD3	1.77	0.46
1:F:366:GLN:HA	1:F:366:GLN:NE2	2.31	0.46
1:B:405:THR:C	1:B:406:HIS:HD2	2.24	0.45
1:D:364:LYS:HA	1:D:367:GLU:OE1	2.15	0.45
1:E:355:ILE:CG1	3:E:6537:HOH:O	2.52	0.45
1:E:497:ASP:OD1	1:E:499:THR:HB	2.17	0.45
1:A:313:LYS:HA	3:A:6607:HOH:O	2.16	0.45
1:D:424:TRP:CH2	1:D:459:PRO:HD3	2.51	0.45
1:E:394:ILE:HD12	3:E:6768:HOH:O	2.15	0.45
1:E:407:LEU:C	3:E:6762:HOH:O	2.58	0.45
1:F:326:ARG:O	1:F:328:ILE:N	2.49	0.45
1:F:382:TYR:N	1:F:382:TYR:CD1	2.84	0.45
1:D:412:VAL:CG2	3:D:6859:HOH:O	2.65	0.45
1:B:425:PRO:HB3	1:B:457:GLN:NE2	2.31	0.45
1:C:365:ARG:NH2	1:C:475:VAL:CG1	2.79	0.45
1:D:424:TRP:NE1	3:D:6860:HOH:O	2.49	0.45
1:D:434:LEU:HB3	1:D:443:VAL:HB	1.99	0.45
1:A:409:LEU:HD23	1:A:409:LEU:C	2.42	0.45
1:A:450:ASP:C	1:A:452:THR:N	2.75	0.45
1:E:478:MET:HA	1:E:482:ASN:OD1	2.17	0.45
1:F:340:GLN:HG3	3:F:6665:HOH:O	2.16	0.45
1:B:450:ASP:O	1:B:452:THR:N	2.50	0.45
1:B:478:MET:C	1:B:480:ALA:H	2.25	0.45
1:C:372:ARG:NE	3:C:6802:HOH:O	2.49	0.45
1:D:444:ILE:HG12	1:D:445:ASP:N	2.32	0.45
1:A:473:CYS:HA	1:A:474:PRO:HD3	1.85	0.45
1:B:365:ARG:NH2	1:B:475:VAL:HG11	2.31	0.45
1:B:418:ASN:ND2	3:B:6490:HOH:O	2.49	0.45
1:D:319:SER:CB	3:D:6482:HOH:O	2.65	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:NH2	3:A:6905:HOH:O	2.50	0.45
1:A:400:GLY:C	1:A:402:GLY:H	2.25	0.44
1:B:486:ARG:NH2	3:B:6584:HOH:O	2.42	0.44
1:E:492:ILE:CG2	3:E:6464:HOH:O	2.65	0.44
1:B:321:VAL:HA	3:B:6452:HOH:O	2.17	0.44
1:B:486:ARG:NH2	3:B:6732:HOH:O	2.50	0.44
1:C:407:LEU:HD23	1:C:407:LEU:C	2.42	0.44
1:F:412:VAL:HG22	1:F:466:ALA:HB2	1.99	0.44
1:F:473:CYS:HA	1:F:474:PRO:HD3	1.79	0.44
1:A:335:MET:HE1	1:C:335:MET:HE3	1.99	0.44
1:A:400:GLY:N	3:A:6763:HOH:O	2.38	0.44
1:C:342:VAL:HG21	3:C:6769:HOH:O	2.16	0.44
1:D:320:LYS:O	1:D:321:VAL:C	2.59	0.44
1:D:360:ASP:HA	1:D:488:ASP:OD2	2.17	0.44
1:D:396:LEU:HD12	3:D:6760:HOH:O	2.17	0.44
1:D:401:THR:O	1:D:471:LEU:HD21	2.18	0.44
1:D:365:ARG:CZ	3:D:6425:HOH:O	2.65	0.44
1:E:389:LYS:C	1:E:390:MET:HG3	2.42	0.44
1:E:451:VAL:HG12	1:E:451:VAL:O	2.16	0.44
1:F:389:LYS:C	1:F:390:MET:HG3	2.43	0.44
1:B:360:ASP:HA	1:B:488:ASP:OD2	2.18	0.44
1:D:365:ARG:NH1	3:D:6425:HOH:O	2.51	0.44
1:E:393:ARG:HA	3:E:6779:HOH:O	2.16	0.44
1:F:443:VAL:CG2	1:F:477:LYS:HE2	2.48	0.44
1:D:417:PRO:HB2	3:D:6577:HOH:O	2.18	0.44
1:E:353:VAL:C	3:E:6410:HOH:O	2.61	0.44
1:A:369:VAL:C	1:A:371:GLY:H	2.26	0.44
1:B:484:TYR:O	1:B:490:ILE:HG22	2.18	0.44
1:E:448:ARG:HB3	3:E:6381:HOH:O	2.18	0.44
1:A:458:ARG:HA	1:A:459:PRO:HD3	1.86	0.43
1:C:342:VAL:HG23	3:C:6769:HOH:O	2.17	0.43
1:C:350:TYR:CD2	1:C:385:ARG:HA	2.52	0.43
1:F:407:LEU:C	1:F:407:LEU:HD23	2.42	0.43
1:A:479:GLU:OE1	1:A:479:GLU:HA	2.19	0.43
1:B:339:GLU:O	1:B:343:LEU:HD13	2.17	0.43
1:E:358:ILE:HD12	1:E:490:ILE:HD11	2.01	0.43
1:D:354:PHE:CE2	1:D:356:TRP:HB2	2.54	0.43
1:E:412:VAL:HG23	3:E:6793:HOH:O	2.18	0.43
1:F:439:ASN:HB3	3:F:6038:HOH:O	2.17	0.43
1:A:406:HIS:ND1	1:A:471:LEU:HD22	2.33	0.43
1:A:482:ASN:N	1:A:482:ASN:ND2	2.65	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:VAL:HG21	3:A:6369:HOH:O	2.19	0.43
1:C:354:PHE:CE2	1:C:356:TRP:HB2	2.54	0.43
1:D:413:VAL:CG1	3:D:6799:HOH:O	2.67	0.43
1:E:394:ILE:HD11	1:E:407:LEU:HD21	2.00	0.43
1:B:409:LEU:HD22	1:B:432:LEU:CD1	2.44	0.43
1:C:409:LEU:HD23	1:C:409:LEU:C	2.44	0.43
1:D:434:LEU:HG	1:D:484:TYR:CD1	2.54	0.43
1:E:356:TRP:CZ3	3:E:6403:HOH:O	2.71	0.43
1:E:407:LEU:C	1:E:407:LEU:HD23	2.43	0.43
1:F:476:SER:C	1:F:478:MET:N	2.76	0.43
1:C:380:ALA:HB1	1:C:414:MET:HE1	1.96	0.43
1:E:363:ARG:HG2	1:E:363:ARG:HH11	1.83	0.43
1:E:340:GLN:O	1:E:344:GLU:HG3	2.19	0.43
1:E:448:ARG:C	3:E:6381:HOH:O	2.61	0.43
1:F:409:LEU:HD23	1:F:409:LEU:C	2.43	0.43
1:F:478:MET:C	1:F:480:ALA:H	2.26	0.43
1:F:479:GLU:OE1	1:F:479:GLU:HA	2.19	0.43
2:G:422:PRO:O	2:G:423:PHE:CD1	2.70	0.43
1:A:401:THR:HG23	3:A:6227:HOH:O	2.18	0.43
1:A:409:LEU:HD23	1:A:410:PHE:N	2.33	0.43
1:A:450:ASP:C	1:A:452:THR:H	2.27	0.43
1:D:358:ILE:C	3:D:6739:HOH:O	2.61	0.43
1:C:382:TYR:CD1	1:C:382:TYR:N	2.87	0.43
1:D:355:ILE:O	3:D:6756:HOH:O	2.22	0.43
1:D:401:THR:HG23	3:D:6736:HOH:O	2.18	0.43
1:A:424:TRP:CH2	1:A:459:PRO:HD3	2.53	0.42
1:C:478:MET:HE2	1:C:485:VAL:CG2	2.49	0.42
1:A:400:GLY:CA	2:G:428:CYS:SG	3.07	0.42
1:E:438:ASN:HB2	1:E:483:SER:HB2	2.01	0.42
1:B:451:VAL:HG23	3:B:6132:HOH:O	2.20	0.42
1:C:398:GLY:CA	1:C:406:HIS:O	2.68	0.42
1:D:350:TYR:HD2	1:D:385:ARG:HA	1.81	0.42
1:D:382:TYR:CZ	1:D:389:LYS:HG3	2.54	0.42
1:D:464:ASN:HB3	3:D:6772:HOH:O	2.18	0.42
1:E:365:ARG:O	1:E:368:ALA:HB3	2.19	0.42
1:E:493:LYS:CB	3:E:6537:HOH:O	2.67	0.42
1:B:344:GLU:CB	3:B:6311:HOH:O	2.67	0.42
1:B:424:TRP:CH2	1:B:459:PRO:HD3	2.55	0.42
1:C:361:PHE:O	1:C:365:ARG:HB2	2.19	0.42
1:C:458:ARG:HA	1:C:459:PRO:HD3	1.80	0.42
1:F:444:ILE:HG12	1:F:445:ASP:N	2.33	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:437:GLN:CD	1:E:486:ARG:HB3	2.44	0.42
1:E:447:PHE:CD1	1:E:447:PHE:C	2.97	0.42
1:A:426:PHE:HB3	1:A:456:PHE:HB3	2.00	0.42
1:F:326:ARG:C	1:F:328:ILE:N	2.78	0.42
1:F:400:GLY:HA3	3:F:6420:HOH:O	2.18	0.42
1:A:320:LYS:O	1:A:323:GLN:N	2.53	0.42
1:B:367:GLU:HG2	1:B:372:ARG:NH2	2.34	0.42
1:E:316:ALA:N	3:E:6892:HOH:O	2.52	0.42
1:B:424:TRP:CG	1:B:458:ARG:HB2	2.55	0.42
1:B:477:LYS:HD2	3:B:6065:HOH:O	2.19	0.42
1:E:493:LYS:CA	3:E:6537:HOH:O	2.54	0.42
1:F:449:PRO:HB3	1:F:456:PHE:CD2	2.55	0.42
2:H:421:VAL:HB	3:H:6569:HOH:O	2.20	0.42
1:B:482:ASN:N	1:B:482:ASN:ND2	2.63	0.41
1:C:434:LEU:HG	1:C:484:TYR:HD2	1.83	0.41
1:F:381:PHE:CE2	1:F:390:MET:HE3	2.55	0.41
1:D:424:TRP:CZ3	1:D:459:PRO:HD3	2.56	0.41
1:F:486:ARG:HG3	1:F:486:ARG:HH11	1.85	0.41
1:A:400:GLY:HA2	2:G:428:CYS:SG	2.60	0.41
1:D:444:ILE:CG1	1:D:445:ASP:N	2.83	0.41
1:F:375:ALA:HB2	1:F:395:TYR:CE2	2.55	0.41
2:G:423:PHE:HD1	2:G:423:PHE:HA	1.76	0.41
1:A:476:SER:C	1:A:478:MET:H	2.27	0.41
1:F:317:LEU:C	3:F:6455:HOH:O	2.63	0.41
1:A:389:LYS:HG2	1:A:414:MET:CE	2.40	0.41
1:B:394:ILE:HD11	1:B:407:LEU:HD21	2.03	0.41
1:B:481:LYS:HG2	3:B:6055:HOH:O	2.21	0.41
1:E:473:CYS:HA	1:E:474:PRO:HD3	1.88	0.41
1:A:443:VAL:HG23	1:A:484:TYR:CE2	2.56	0.41
1:E:316:ALA:N	3:E:6646:HOH:O	2.54	0.41
1:E:356:TRP:CE2	3:E:6403:HOH:O	2.74	0.41
1:A:486:ARG:HD2	3:A:6320:HOH:O	2.21	0.41
1:B:386:TYR:CZ	1:C:355:ILE:HB	2.55	0.41
1:B:450:ASP:C	1:B:452:THR:N	2.78	0.41
1:F:436:ASP:C	1:F:438:ASN:H	2.26	0.41
1:B:407:LEU:HD23	1:B:407:LEU:C	2.46	0.41
1:C:393:ARG:NH2	3:C:6405:HOH:O	2.52	0.41
1:E:338:LEU:O	1:E:341:LYS:HB3	2.20	0.41
1:A:400:GLY:C	1:A:402:GLY:N	2.79	0.41
1:A:416:GLY:HA3	3:A:6079:HOH:O	2.20	0.41
1:A:436:ASP:OD1	1:A:438:ASN:HB2	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:SER:OG	2:G:424:SER:HB2	2.21	0.41
1:A:469:CYS:HA	1:A:470:PRO:HD2	1.97	0.41
1:B:475:VAL:C	1:B:477:LYS:N	2.79	0.41
1:C:372:ARG:HH11	1:C:372:ARG:HD3	1.76	0.41
1:D:324:LEU:C	1:D:326:ARG:H	2.29	0.41
1:E:399:ASP:O	1:E:400:GLY:C	2.64	0.41
1:E:409:LEU:C	1:E:409:LEU:CD2	2.94	0.41
1:E:458:ARG:HA	1:E:459:PRO:HD3	1.92	0.41
1:E:318:SER:N	3:E:6646:HOH:O	2.53	0.41
1:A:313:LYS:N	3:A:6501:HOH:O	2.53	0.40
1:A:388:TYR:CD2	1:A:422:LEU:HD23	2.55	0.40
1:B:436:ASP:C	1:B:438:ASN:N	2.79	0.40
1:D:345:MET:SD	1:E:342:VAL:HG13	2.61	0.40
1:D:448:ARG:HA	1:D:449:PRO:HD3	1.88	0.40
1:E:373:ILE:HB	3:E:6825:HOH:O	2.21	0.40
1:E:393:ARG:N	3:E:6780:HOH:O	2.52	0.40
1:E:393:ARG:CG	3:E:6779:HOH:O	2.56	0.40
1:E:477:LYS:O	1:E:477:LYS:HG2	2.21	0.40
1:A:405:THR:HG22	1:E:463:MET:HE3	2.03	0.40
1:A:421:LEU:HD11	1:B:491:PHE:CD2	2.57	0.40
1:A:422:LEU:HD12	1:A:422:LEU:N	2.37	0.40
1:C:405:THR:C	1:C:406:HIS:HD2	2.28	0.40
1:D:337:ASP:CB	3:D:6843:HOH:O	2.69	0.40
1:A:339:GLU:O	1:A:343:LEU:HD13	2.21	0.40
1:C:365:ARG:NH2	1:C:475:VAL:HG11	2.36	0.40
1:E:338:LEU:HD21	1:F:342:VAL:HG21	2.03	0.40
1:E:389:LYS:HE2	1:E:414:MET:CE	2.51	0.40
1:D:413:VAL:HG13	3:D:6799:HOH:O	2.20	0.40
1:E:391:CYS:SG	1:E:412:VAL:HB	2.61	0.40
1:A:337:ASP:CB	3:A:6748:HOH:O	2.70	0.40
1:D:357:LYS:CG	3:D:6739:HOH:O	2.66	0.40
1:F:401:THR:HG23	3:F:6420:HOH:O	2.21	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	189/192 (98%)	174 (92%)	13 (7%)	2 (1%)	11	13
1	B	189/192 (98%)	175 (93%)	11 (6%)	3 (2%)	7	7
1	C	189/192 (98%)	183 (97%)	6 (3%)	0	100	100
1	D	184/192 (96%)	166 (90%)	17 (9%)	1 (0%)	24	31
1	E	184/192 (96%)	167 (91%)	14 (8%)	3 (2%)	7	7
1	F	184/192 (96%)	169 (92%)	12 (6%)	3 (2%)	7	7
2	G	5/10 (50%)	5 (100%)	0	0	100	100
2	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	1132/1172 (97%)	1046 (92%)	74 (6%)	12 (1%)	11	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	401	THR
1	A	451	VAL
1	B	451	VAL
1	B	479	GLU
1	F	327	SER
1	E	439	ASN
1	B	439	ASN
1	E	478	MET
1	F	477	LYS
1	A	401	THR
1	F	478	MET
1	D	451	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	Percentiles	
1	A	145/166 (87%)	143 (99%)	2 (1%)	59	76
1	B	138/166 (83%)	136 (99%)	2 (1%)	59	76
1	C	145/166 (87%)	141 (97%)	4 (3%)	38	56
1	D	141/166 (85%)	137 (97%)	4 (3%)	38	56
1	E	143/166 (86%)	140 (98%)	3 (2%)	47	66
1	F	140/166 (84%)	135 (96%)	5 (4%)	31	47
2	G	7/9 (78%)	6 (86%)	1 (14%)	3	3
2	H	9/9 (100%)	9 (100%)	0	100	100
All	All	868/1014 (86%)	847 (98%)	21 (2%)	43	62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	ASN
1	A	482	ASN
1	B	422	LEU
1	B	482	ASN
1	C	335	MET
1	C	365	ARG
1	C	407	LEU
1	C	438	ASN
1	D	335	MET
1	D	422	LEU
1	D	438	ASN
1	D	482	ASN
1	E	338	LEU
1	E	438	ASN
1	E	482	ASN
1	F	340	GLN
1	F	343	LEU
1	F	409	LEU
1	F	438	ASN
1	F	482	ASN
2	G	423	PHE

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

Mol	Chain	Res	Type
1	A	427	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	439	ASN
1	A	461	ASN
1	A	482	ASN
1	B	397	ASN
1	B	406	HIS
1	B	438	ASN
1	B	439	ASN
1	B	461	ASN
1	B	482	ASN
1	C	366	GLN
1	C	428	GLN
1	D	418	ASN
1	D	427	ASN
1	D	439	ASN
1	D	457	GLN
1	D	461	ASN
1	D	482	ASN
1	E	397	ASN
1	E	438	ASN
1	E	461	ASN
1	F	366	GLN
1	F	438	ASN
1	F	461	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 oligosaccharides 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

### 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.