



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:48 pm GMT

PDB ID : 2VF1  
Title : X-RAY CRYSTALLOGRAPHIC STRUCTURE OF THE PICOBIR-NAVIRUS CAPSID  
Authors : Duquerroy, S.; Da Costa, B.; Vigouroux, A.; Lepault, J.; Navaza, J.; Delmas, B.; Rey, F.A.  
Deposited on : 2007-10-29  
Resolution : 3.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

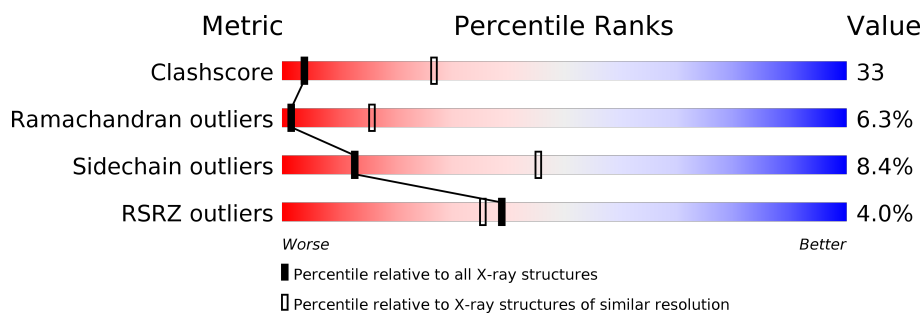
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	525	<div> <div>4%</div> <div>50%</div> <div>41%</div> <div>8%</div> </div>
1	B	525	<div> <div>4%</div> <div>50%</div> <div>40%</div> <div>9%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8286 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 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4117	2634	671	794	18			
1	B	525	Total	C	N	O	S	0	0	0
			4117	2634	671	794	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	TYR	UNK	SEE REMARK 999	UNP Q9Q1V2
B	179	TYR	UNK	SEE REMARK 999	UNP Q9Q1V2

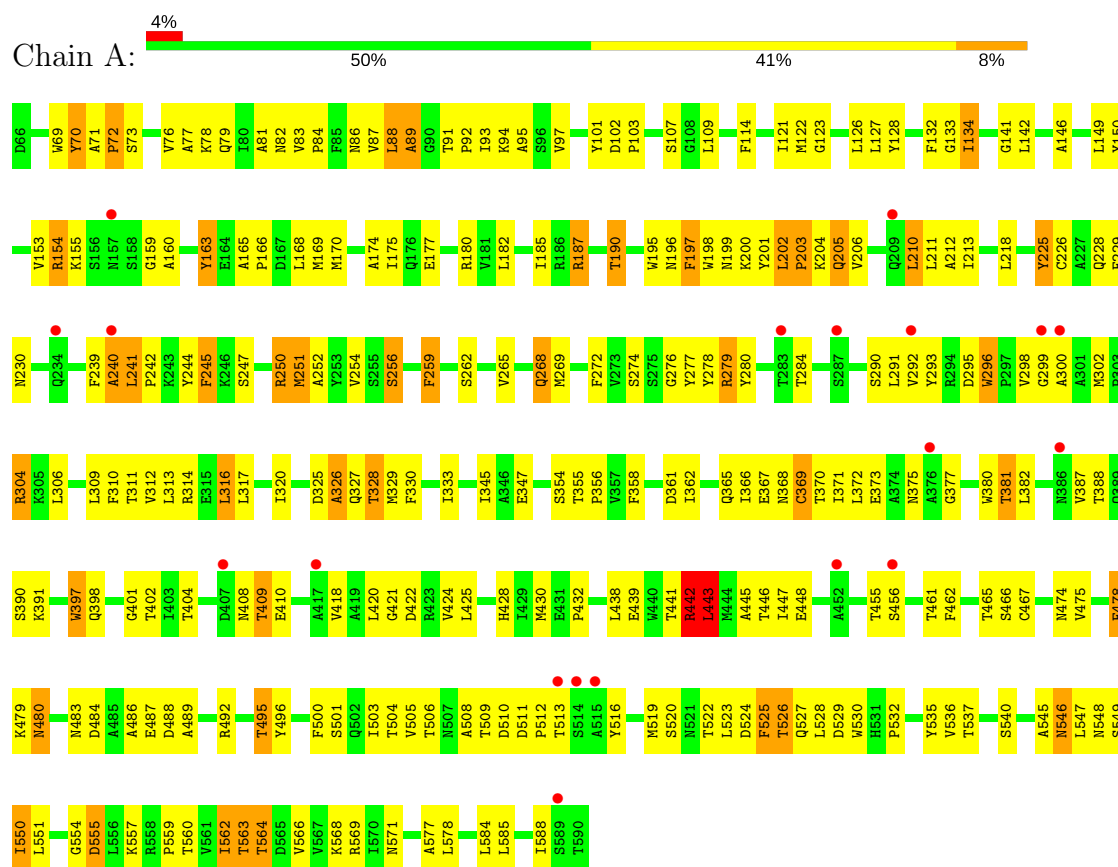
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	30	Total	O	0	0
			30	30		

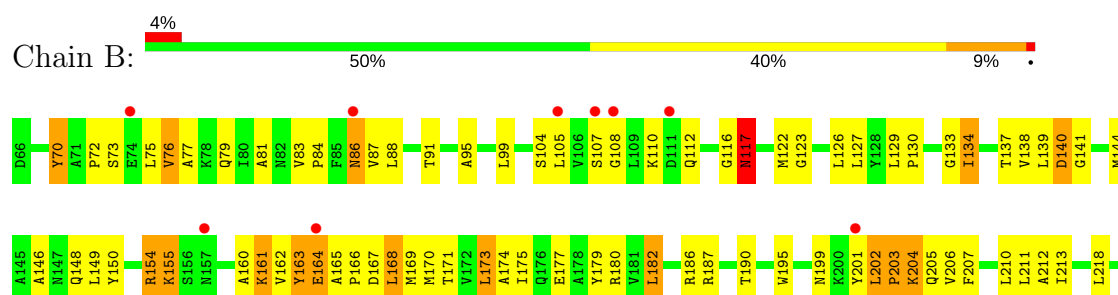
### 3 Residue-property plots

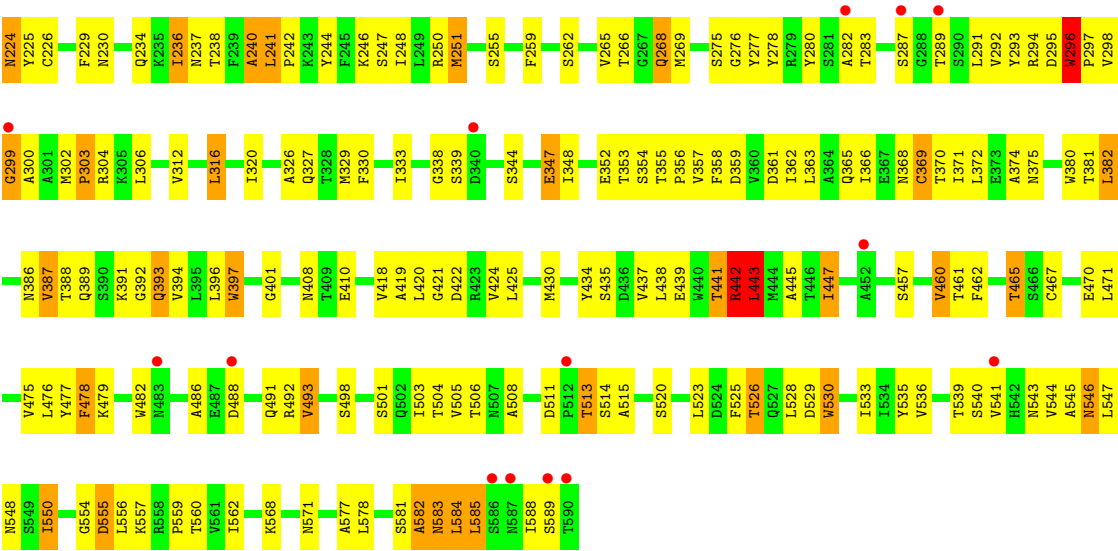
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: CAPSID PROTEIN



#### • Molecule 1: CAPSID PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	407.42Å 407.42Å 808.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.98 – 3.40 78.82 – 3.40	Depositor EDS
% Data completeness (in resolution range)	70.0 (49.98-3.40) 43.5 (78.82-3.40)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.273 , 0.272 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , -69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.087 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.41	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0/4209	0.72	1/5737 (0.0%)
1	B	0.47	0/4209	0.73	2/5737 (0.0%)
All	All	0.47	0/8418	0.72	3/11474 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	LEU	N-CA-C	-5.40	96.41	111.00
1	B	443	LEU	N-CA-C	-5.32	96.64	111.00
1	B	296	TRP	C-N-CD	5.13	139.17	128.40

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	4117	0	4038	281	0
1	B	4117	0	4038	302	0
2	A	22	0	0	2	0
2	B	30	0	0	0	0
All	All	8286	0	8076	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 33.

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:72:PRO:HG2	1:B:76:VAL:HG11	1.34	1.05
1:B:419:ALA:HB1	1:B:447:ILE:HD13	1.40	1.03
1:A:187:ARG:HH11	1:A:187:ARG:HG2	1.26	0.99
1:A:442:ARG:N	1:A:442:ARG:HH11	1.62	0.97
1:A:381:THR:HG22	1:A:402:THR:H	1.30	0.96
1:B:442:ARG:HH11	1:B:442:ARG:N	1.61	0.96
1:A:174:ALA:HB1	1:A:320:ILE:HD12	1.47	0.95
1:A:70:TYR:HB2	1:B:438:LEU:HD21	1.51	0.92
1:A:557:LYS:HE3	1:B:262:SER:HB2	1.51	0.92
1:B:73:SER:HB3	1:B:76:VAL:HG12	1.52	0.91
1:A:252:ALA:O	1:A:256:SER:HB2	1.71	0.91
1:A:424:VAL:HG12	1:A:535:TYR:OH	1.70	0.91
1:A:247:SER:HA	1:A:578:LEU:HD22	1.51	0.91
1:B:424:VAL:HG12	1:B:535:TYR:OH	1.70	0.91
1:A:298:VAL:HG13	1:A:299:GLY:H	1.35	0.90
1:B:88:LEU:H	1:B:88:LEU:HD12	1.38	0.89
1:B:278:TYR:O	1:B:316:LEU:HD21	1.74	0.86
1:B:148:GLN:HE21	1:B:582:ALA:H	1.23	0.85
1:B:442:ARG:CZ	1:B:442:ARG:HB2	2.04	0.85
1:A:88:LEU:HD13	1:A:200:LYS:HE3	1.56	0.85
1:B:418:VAL:HG11	1:B:503:ILE:HG21	1.59	0.85
1:B:160:ALA:O	1:B:162:VAL:HG23	1.77	0.84
1:A:218:LEU:HD13	1:A:306:LEU:HD12	1.57	0.84
1:B:291:LEU:HB2	1:B:387:VAL:CG1	2.08	0.83
1:B:291:LEU:HB2	1:B:387:VAL:HG13	1.60	0.83
1:A:442:ARG:HB2	1:A:442:ARG:CZ	2.08	0.82
1:B:187:ARG:HD3	1:B:211:LEU:HD23	1.61	0.82
1:A:87:VAL:HG11	1:B:560:THR:HA	1.60	0.82
1:B:381:THR:HG22	1:B:382:LEU:H	1.44	0.82
1:A:381:THR:HG22	1:A:402:THR:N	1.93	0.81
1:A:163:TYR:HD2	1:A:163:TYR:N	1.77	0.81
1:A:187:ARG:NH1	1:A:211:LEU:HD22	1.95	0.81
1:A:121:ILE:HD11	1:A:524:ASP:HB3	1.61	0.80
1:A:268:GLN:H	1:A:268:GLN:CD	1.82	0.80
1:A:420:LEU:H	1:A:420:LEU:HD23	1.48	0.79
1:B:247:SER:HA	1:B:578:LEU:HD22	1.63	0.79
1:A:268:GLN:HG3	1:A:528:LEU:HD23	1.65	0.79
1:B:244:TYR:OH	1:B:581:SER:HB3	1.81	0.79
1:B:169:MET:O	1:B:173:LEU:HD12	1.83	0.78
1:A:163:TYR:N	1:A:163:TYR:CD2	2.48	0.78

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:HD13	1:A:239:PHE:HB3	1.67	0.76
1:B:268:GLN:CD	1:B:268:GLN:H	1.89	0.75
1:B:441:THR:HG22	1:B:442:ARG:N	2.01	0.74
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.68	0.74
1:B:368:ASN:OD1	1:B:425:LEU:HD12	1.87	0.74
1:A:187:ARG:NH1	1:A:187:ARG:HG2	2.03	0.73
1:A:442:ARG:N	1:A:442:ARG:NH1	2.36	0.73
1:B:88:LEU:O	1:B:91:THR:HG23	1.89	0.73
1:B:508:ALA:HB3	1:B:520:SER:HB3	1.68	0.73
1:A:430:MET:CE	1:B:265:VAL:H	2.02	0.73
1:B:150:TYR:CD2	1:B:165:ALA:HA	2.24	0.72
1:B:174:ALA:HB1	1:B:320:ILE:HD12	1.72	0.72
1:B:187:ARG:HD3	1:B:211:LEU:CD2	2.18	0.72
1:A:202:LEU:O	1:A:203:PRO:C	2.28	0.72
1:A:146:ALA:HB2	1:A:169:MET:HG2	1.72	0.72
1:A:430:MET:HE1	1:B:265:VAL:H	1.56	0.71
1:A:296:TRP:HH2	1:A:312:VAL:HG11	1.55	0.71
1:A:265:VAL:H	1:B:430:MET:CE	2.03	0.71
1:A:276:GLY:HA3	1:A:293:TYR:HE1	1.56	0.71
1:B:442:ARG:H	1:B:442:ARG:HD3	1.55	0.71
1:A:442:ARG:HD3	1:A:442:ARG:H	1.56	0.71
1:B:442:ARG:NH1	1:B:442:ARG:N	2.39	0.71
1:B:447:ILE:H	1:B:447:ILE:HD12	1.55	0.70
1:B:296:TRP:O	1:B:298:VAL:N	2.25	0.70
1:A:87:VAL:CG1	1:B:560:THR:HA	2.22	0.69
1:A:370:THR:HG23	1:A:420:LEU:HD21	1.74	0.69
1:B:175:ILE:HG21	1:B:241:LEU:HB2	1.74	0.69
1:B:370:THR:HG23	1:B:420:LEU:HD21	1.74	0.69
1:A:298:VAL:HG13	1:A:299:GLY:N	2.08	0.69
1:B:88:LEU:N	1:B:88:LEU:HD12	2.07	0.69
1:A:375:ASN:HA	1:A:501:SER:HB3	1.73	0.68
1:B:202:LEU:O	1:B:203:PRO:C	2.30	0.68
1:B:381:THR:HG22	1:B:382:LEU:N	2.07	0.68
1:B:465:THR:HG21	1:B:568:LYS:HE2	1.74	0.68
1:B:504:THR:CG2	1:B:536:VAL:HG22	2.24	0.67
1:A:81:ALA:O	1:A:83:VAL:HG23	1.95	0.67
1:A:212:ALA:O	1:A:213:ILE:HD13	1.95	0.67
1:A:540:SER:N	1:A:548:ASN:HB3	2.10	0.66
1:A:202:LEU:HD23	1:A:206:VAL:HG21	1.77	0.66
1:A:549:SER:CB	1:B:117:ASN:HB3	2.26	0.66
1:B:488:ASP:HB3	1:B:491:GLN:HB2	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:CYS:SG	1:B:348:ILE:HD11	2.36	0.66
1:A:313:LEU:O	1:A:317:LEU:HD12	1.95	0.66
1:A:239:PHE:HA	1:A:330:PHE:CE2	2.31	0.66
1:A:89:ALA:CB	1:A:199:ASN:HA	2.26	0.66
1:A:154:ARG:NH2	1:A:159:GLY:O	2.29	0.65
1:B:556:LEU:HD22	1:B:559:PRO:HB3	1.78	0.65
1:A:368:ASN:OD1	1:A:425:LEU:HD12	1.97	0.65
1:A:296:TRP:O	1:A:298:VAL:N	2.30	0.65
1:B:179:TYR:CE1	1:B:236:ILE:HD12	2.32	0.65
1:A:240:ALA:HB1	1:A:333:ILE:HG21	1.79	0.65
1:A:265:VAL:H	1:B:430:MET:HE1	1.62	0.65
1:B:225:TYR:CE1	1:B:306:LEU:HB2	2.32	0.65
1:B:302:MET:HE1	1:B:303:PRO:HD2	1.78	0.64
1:B:276:GLY:HA3	1:B:293:TYR:CE1	2.33	0.64
1:B:163:TYR:N	1:B:163:TYR:CD2	2.66	0.64
1:B:73:SER:HB3	1:B:76:VAL:CG1	2.25	0.64
1:B:87:VAL:HG13	1:B:87:VAL:O	1.97	0.64
1:A:89:ALA:HB2	1:A:199:ASN:HA	1.80	0.64
1:A:326:ALA:O	1:A:329:MET:HB2	1.96	0.64
1:B:543:ASN:ND2	1:B:545:ALA:HB3	2.12	0.63
1:B:420:LEU:H	1:B:420:LEU:HD23	1.62	0.63
1:A:438:LEU:HD21	1:B:70:TYR:HB2	1.80	0.63
1:A:550:ILE:HG23	1:B:116:GLY:HA2	1.79	0.63
1:B:170:MET:SD	1:B:291:LEU:HD13	2.38	0.63
1:B:581:SER:O	1:B:583:ASN:N	2.31	0.63
1:A:504:THR:CG2	1:A:536:VAL:HG22	2.28	0.63
1:B:122:MET:HB2	1:B:201:TYR:CE2	2.34	0.63
1:A:441:THR:HG22	1:A:442:ARG:N	2.14	0.63
1:A:87:VAL:HG13	1:A:87:VAL:O	1.97	0.63
1:B:543:ASN:HD21	1:B:545:ALA:HB3	1.62	0.63
1:A:174:ALA:HB1	1:A:320:ILE:CD1	2.25	0.62
1:A:174:ALA:CB	1:A:320:ILE:HD12	2.27	0.62
1:A:529:ASP:O	1:A:530:TRP:HB2	1.99	0.62
1:B:212:ALA:O	1:B:213:ILE:HD13	2.00	0.62
1:B:540:SER:N	1:B:548:ASN:HB3	2.14	0.62
1:A:122:MET:HB2	1:A:201:TYR:CE2	2.35	0.62
1:B:207:PHE:HA	1:B:211:LEU:HD13	1.80	0.62
1:B:162:VAL:O	1:B:162:VAL:HG12	2.00	0.62
1:A:557:LYS:HE3	1:B:262:SER:CB	2.29	0.62
1:A:205:GLN:NE2	1:A:480:ASN:ND2	2.48	0.62
1:A:577:ALA:HB2	1:B:72:PRO:HD3	1.80	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ALA:HB3	1:A:520:SER:HB3	1.81	0.61
1:A:88:LEU:CD1	1:A:200:LYS:HE3	2.31	0.61
1:B:424:VAL:HG22	1:B:425:LEU:N	2.16	0.61
1:B:529:ASP:O	1:B:530:TRP:HB2	1.99	0.61
1:B:99:LEU:HD12	1:B:99:LEU:O	2.00	0.61
1:B:180:ARG:N	1:B:251:MET:HE1	2.16	0.61
1:A:584:LEU:HG	1:A:585:LEU:CD1	2.29	0.61
1:B:276:GLY:HA3	1:B:293:TYR:HE1	1.66	0.61
1:B:268:GLN:HG3	1:B:528:LEU:HD23	1.82	0.60
1:A:276:GLY:HA3	1:A:293:TYR:CE1	2.36	0.60
1:B:355:THR:HG23	1:B:356:PRO:HD2	1.83	0.60
1:B:441:THR:HB	1:B:442:ARG:HD3	1.83	0.60
1:B:99:LEU:O	1:B:112:GLN:HB3	2.01	0.60
1:A:259:PHE:CD1	1:A:259:PHE:N	2.69	0.60
1:B:259:PHE:CE2	1:B:362:ILE:HG13	2.36	0.59
1:B:504:THR:HG23	1:B:536:VAL:HG22	1.83	0.59
1:B:126:LEU:HD11	1:B:366:ILE:HD12	1.85	0.59
1:B:418:VAL:CG1	1:B:503:ILE:HG21	2.31	0.59
1:A:489:ALA:HA	1:A:492:ARG:HE	1.67	0.59
1:B:211:LEU:N	1:B:211:LEU:HD12	2.18	0.59
1:B:138:VAL:HG22	1:B:394:VAL:HG21	1.85	0.58
1:B:129:LEU:HB3	1:B:471:LEU:HD23	1.84	0.58
1:B:434:TYR:CD1	1:B:435:SER:N	2.71	0.58
1:B:88:LEU:H	1:B:88:LEU:CD1	2.13	0.58
1:B:326:ALA:O	1:B:329:MET:HB2	2.02	0.58
1:A:132:PHE:HB3	1:A:142:LEU:HD21	1.85	0.58
1:A:259:PHE:CE2	1:A:362:ILE:HG13	2.39	0.58
1:A:555:ASP:OD1	1:B:529:ASP:HB2	2.03	0.58
1:A:442:ARG:HH11	1:A:442:ARG:H	1.49	0.58
1:A:418:VAL:HG23	1:A:503:ILE:HD12	1.86	0.57
1:B:117:ASN:ND2	1:B:482:TRP:O	2.38	0.57
1:B:138:VAL:HA	1:B:394:VAL:HG22	1.85	0.57
1:B:535:TYR:HD2	1:B:550:ILE:HD11	1.70	0.57
1:B:84:PRO:HG2	1:B:86:ASN:ND2	2.20	0.57
1:A:560:THR:HA	1:B:87:VAL:HG11	1.86	0.57
1:B:442:ARG:HG3	1:B:571:ASN:OD1	2.05	0.57
1:A:381:THR:HG21	1:A:402:THR:HG23	1.87	0.57
1:B:146:ALA:HA	1:B:169:MET:HE2	1.87	0.57
1:A:84:PRO:HB2	1:A:86:ASN:ND2	2.20	0.56
1:B:162:VAL:C	1:B:163:TYR:HD2	2.08	0.56
1:B:179:TYR:CZ	1:B:236:ILE:HG23	2.40	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TYR:O	1:A:316:LEU:HD21	2.05	0.56
1:A:277:TYR:O	1:A:293:TYR:HD1	1.87	0.56
1:A:239:PHE:HA	1:A:330:PHE:HE2	1.71	0.56
1:B:163:TYR:CE1	1:B:329:MET:HG2	2.40	0.56
1:B:460:VAL:O	1:B:460:VAL:HG12	2.05	0.56
1:A:72:PRO:HG2	1:A:73:SER:H	1.69	0.56
1:B:302:MET:CE	1:B:303:PRO:HD2	2.36	0.56
1:A:478:PHE:N	1:A:478:PHE:CD1	2.74	0.56
1:A:409:THR:HG22	1:A:409:THR:O	2.06	0.55
1:A:121:ILE:HD12	1:A:527:GLN:HB2	1.89	0.55
1:B:244:TYR:CZ	1:B:581:SER:HB3	2.41	0.55
1:B:180:ARG:HB2	1:B:251:MET:HE2	1.87	0.55
1:B:73:SER:CB	1:B:76:VAL:HG12	2.31	0.55
1:A:496:TYR:CD2	1:B:544:VAL:HG21	2.40	0.55
1:A:529:ASP:HB2	1:B:555:ASP:OD1	2.06	0.55
1:A:122:MET:CE	1:A:210:LEU:HD22	2.37	0.55
1:B:268:GLN:CD	1:B:268:GLN:N	2.59	0.55
1:B:174:ALA:HB1	1:B:320:ILE:CD1	2.36	0.55
1:A:196:ASN:O	1:A:198:TRP:N	2.39	0.55
1:A:424:VAL:HG22	1:A:425:LEU:N	2.22	0.55
1:B:478:PHE:N	1:B:478:PHE:CD1	2.74	0.55
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.89	0.55
1:B:259:PHE:CD1	1:B:259:PHE:N	2.75	0.55
1:A:274:SER:O	1:A:296:TRP:HD1	1.90	0.54
1:A:512:PRO:HD3	1:A:519:MET:HE1	1.88	0.54
1:B:190:THR:HG22	1:B:354:SER:H	1.73	0.54
1:B:230:ASN:OD1	1:B:347:GLU:HB3	2.07	0.54
1:B:180:ARG:NH1	1:B:251:MET:HB2	2.23	0.54
1:B:316:LEU:O	1:B:320:ILE:HG12	2.07	0.54
1:B:442:ARG:CB	1:B:442:ARG:CZ	2.83	0.54
1:A:168:LEU:C	1:A:168:LEU:HD23	2.27	0.54
1:A:421:GLY:HA2	1:A:564:THR:HG23	1.89	0.54
1:A:251:MET:HG3	1:A:252:ALA:N	2.23	0.54
1:A:127:LEU:HD23	1:A:474:ASN:HD21	1.73	0.54
1:B:149:LEU:HD23	1:B:149:LEU:C	2.29	0.54
1:B:582:ALA:C	1:B:584:LEU:H	2.12	0.54
1:B:375:ASN:HA	1:B:501:SER:HB3	1.90	0.53
1:A:163:TYR:CE1	1:A:329:MET:HG2	2.44	0.53
1:A:551:LEU:CD2	1:B:479:LYS:HE3	2.38	0.53
1:B:365:GLN:HB3	1:B:443:LEU:HD22	1.90	0.53
1:A:387:VAL:HG22	1:A:397:TRP:HB2	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:HD2	1:B:164:GLU:OE2	2.09	0.53
1:B:240:ALA:HB1	1:B:333:ILE:HD12	1.90	0.53
1:A:448:GLU:HB2	1:A:465:THR:HG23	1.89	0.53
1:B:163:TYR:N	1:B:163:TYR:HD2	2.06	0.53
1:B:348:ILE:HG13	1:B:348:ILE:O	2.09	0.53
1:B:418:VAL:HG11	1:B:503:ILE:CG2	2.34	0.53
1:A:560:THR:HA	1:B:87:VAL:CG1	2.39	0.53
1:B:237:ASN:OD1	1:B:344:SER:HA	2.08	0.53
1:A:465:THR:HB	1:A:568:LYS:HE2	1.91	0.53
1:A:218:LEU:HD12	1:A:225:TYR:HD1	1.74	0.53
1:A:438:LEU:CD2	1:B:70:TYR:HB2	2.38	0.53
1:A:109:LEU:N	1:A:109:LEU:HD23	2.24	0.52
1:A:430:MET:HE1	1:B:265:VAL:N	2.23	0.52
1:B:370:THR:HB	1:B:445:ALA:H	1.74	0.52
1:B:190:THR:HG22	1:B:354:SER:N	2.25	0.52
1:A:371:ILE:HD12	1:A:475:VAL:CG2	2.40	0.52
1:A:182:LEU:HD13	1:A:345:ILE:HD11	1.91	0.52
1:A:355:THR:HG23	1:A:356:PRO:HD2	1.92	0.52
1:B:387:VAL:HA	1:B:396:LEU:O	2.10	0.52
1:B:465:THR:HG21	1:B:568:LYS:CE	2.39	0.52
1:A:496:TYR:CG	1:B:544:VAL:HG21	2.45	0.52
1:B:137:THR:HG22	1:B:138:VAL:N	2.25	0.52
1:A:420:LEU:CD2	1:A:420:LEU:H	2.21	0.51
1:B:470:GLU:O	1:B:471:LEU:HB3	2.10	0.51
1:A:149:LEU:HD13	1:A:149:LEU:C	2.30	0.51
1:B:72:PRO:HG2	1:B:76:VAL:CG1	2.23	0.51
1:A:146:ALA:N	1:A:169:MET:HE3	2.25	0.51
1:A:205:GLN:HE22	1:A:480:ASN:ND2	2.07	0.51
1:A:504:THR:HG23	1:A:536:VAL:HG22	1.93	0.51
1:B:486:ALA:HB3	1:B:492:ARG:NH2	2.26	0.51
1:A:268:GLN:CD	1:A:268:GLN:N	2.59	0.51
1:B:130:PRO:HB2	1:B:278:TYR:HE1	1.75	0.51
1:B:234:GLN:O	1:B:238:THR:HG23	2.10	0.51
1:B:81:ALA:O	1:B:83:VAL:N	2.44	0.51
1:A:265:VAL:H	1:B:430:MET:HE2	1.73	0.51
1:B:122:MET:HB2	1:B:201:TYR:CD2	2.45	0.51
1:B:442:ARG:H	1:B:442:ARG:CD	2.21	0.51
1:B:371:ILE:HD12	1:B:475:VAL:CG2	2.41	0.51
1:B:146:ALA:HA	1:B:169:MET:CE	2.41	0.51
1:B:199:ASN:OD1	1:B:201:TYR:HB2	2.11	0.51
1:B:154:ARG:HG2	1:B:154:ARG:HH11	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:O	1:B:77:ALA:N	2.44	0.50
1:A:300:ALA:HA	2:A:2013:HOH:O	2.11	0.50
1:B:282:ALA:HB2	1:B:289:THR:HG22	1.93	0.50
1:B:424:VAL:HG12	1:B:535:TYR:HH	1.75	0.50
1:A:226:CYS:O	1:A:229:PHE:HB3	2.12	0.50
1:A:377:GLY:HA2	1:A:519:MET:HE3	1.93	0.50
1:A:73:SER:OG	1:A:76:VAL:HG23	2.11	0.50
1:B:187:ARG:NH2	1:B:255:SER:HA	2.26	0.50
1:A:442:ARG:CB	1:A:442:ARG:CZ	2.86	0.50
1:B:137:THR:C	1:B:139:LEU:H	2.14	0.50
1:B:148:GLN:HE21	1:B:582:ALA:N	2.00	0.50
1:B:372:LEU:O	1:B:374:ALA:N	2.44	0.50
1:A:317:LEU:HA	1:A:320:ILE:HG12	1.92	0.50
1:A:325:ASP:O	1:A:328:THR:HG23	2.11	0.50
1:A:408:ASN:C	1:A:410:GLU:H	2.15	0.50
1:A:150:TYR:CD2	1:A:165:ALA:HA	2.47	0.50
1:A:163:TYR:HD2	1:A:163:TYR:H	1.54	0.50
1:B:442:ARG:H	1:B:442:ARG:HH11	1.52	0.50
1:B:182:LEU:CD2	1:B:229:PHE:CE1	2.95	0.50
1:A:182:LEU:HD21	1:A:229:PHE:CE1	2.47	0.50
1:A:442:ARG:CD	1:A:442:ARG:H	2.22	0.50
1:A:445:ALA:HB1	1:A:466:SER:O	2.12	0.50
1:B:486:ALA:CB	1:B:492:ARG:CZ	2.90	0.50
1:A:240:ALA:H	1:A:330:PHE:HD2	1.58	0.49
1:A:424:VAL:HG12	1:A:535:TYR:CZ	2.48	0.49
1:B:280:TYR:HB2	1:B:320:ILE:HD13	1.94	0.49
1:B:148:GLN:NE2	1:B:582:ALA:H	2.00	0.49
1:A:175:ILE:CD1	1:A:239:PHE:HB3	2.39	0.49
1:B:424:VAL:HG11	1:B:533:ILE:HG21	1.93	0.49
1:A:279:ARG:O	1:A:291:LEU:HD12	2.12	0.49
1:A:163:TYR:CD1	1:A:329:MET:HG2	2.47	0.49
1:B:186:ARG:HD2	1:B:229:PHE:CZ	2.48	0.49
1:B:442:ARG:CA	1:B:442:ARG:NH1	2.75	0.49
1:B:122:MET:HE3	1:B:210:LEU:HG	1.95	0.49
1:A:149:LEU:O	1:A:153:VAL:HG23	2.12	0.49
1:B:218:LEU:HD12	1:B:218:LEU:O	2.13	0.49
1:B:155:LYS:HZ3	1:B:588:ILE:HB	1.78	0.49
1:A:123:GLY:HA3	1:A:269:MET:O	2.12	0.49
1:A:187:ARG:HH12	1:A:211:LEU:HD22	1.77	0.49
1:A:408:ASN:O	1:A:410:GLU:N	2.45	0.49
1:B:540:SER:H	1:B:548:ASN:HB3	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:TRP:CH2	1:A:312:VAL:HG11	2.43	0.49
1:A:312:VAL:HG13	1:A:313:LEU:N	2.28	0.49
1:B:298:VAL:HG13	1:B:299:GLY:N	2.27	0.49
1:B:540:SER:HB2	1:B:546:ASN:O	2.13	0.49
1:A:480:ASN:HB3	1:A:495:THR:HA	1.95	0.49
1:A:206:VAL:HG13	1:A:210:LEU:HD23	1.95	0.48
1:A:212:ALA:C	1:A:213:ILE:HD13	2.33	0.48
1:A:422:ASP:OD1	1:A:563:THR:HA	2.12	0.48
1:A:121:ILE:HG23	1:A:478:PHE:O	2.13	0.48
1:A:311:THR:HG23	1:A:314:ARG:NH1	2.28	0.48
1:A:446:THR:CG2	1:A:564:THR:HG22	2.43	0.48
1:A:291:LEU:HB3	1:A:387:VAL:HB	1.94	0.48
1:A:177:GLU:O	1:A:180:ARG:HB3	2.14	0.48
1:A:368:ASN:O	1:A:369:CYS:O	2.32	0.48
1:A:445:ALA:HB2	1:A:467:CYS:CB	2.44	0.48
1:B:280:TYR:CB	1:B:320:ILE:HD13	2.43	0.48
1:B:248:ILE:O	1:B:251:MET:HG3	2.13	0.48
1:A:265:VAL:N	1:B:430:MET:HE1	2.27	0.48
1:A:277:TYR:CE2	1:A:312:VAL:HG21	2.49	0.48
1:A:296:TRP:HA	1:A:296:TRP:CE3	2.48	0.48
1:A:505:VAL:HG12	1:A:506:THR:N	2.28	0.48
1:A:91:THR:HB	1:A:92:PRO:HD2	1.95	0.48
1:B:186:ARG:HD2	1:B:229:PHE:HZ	1.78	0.48
1:B:381:THR:CG2	1:B:382:LEU:H	2.20	0.48
1:A:262:SER:HB3	1:B:557:LYS:HE2	1.96	0.48
1:A:155:LYS:HE3	1:A:588:ILE:HG23	1.95	0.47
1:A:196:ASN:O	1:A:197:PHE:C	2.51	0.47
1:A:316:LEU:O	1:A:320:ILE:HG12	2.14	0.47
1:A:89:ALA:HB3	1:A:199:ASN:HA	1.96	0.47
1:B:84:PRO:CG	1:B:86:ASN:ND2	2.77	0.47
1:A:365:GLN:C	1:A:443:LEU:HD23	2.35	0.47
1:A:441:THR:O	1:A:443:LEU:N	2.47	0.47
1:B:424:VAL:HG12	1:B:535:TYR:CZ	2.48	0.47
1:B:511:ASP:HB3	1:B:513:THR:OG1	2.15	0.47
1:A:545:ALA:C	1:A:547:LEU:H	2.18	0.47
1:B:212:ALA:O	1:B:304:ARG:HG2	2.14	0.47
1:A:133:GLY:O	1:A:134:ILE:C	2.52	0.47
1:A:522:THR:O	1:A:524:ASP:N	2.48	0.47
1:A:204:LYS:O	1:A:206:VAL:N	2.48	0.47
1:B:225:TYR:CD1	1:B:306:LEU:HD12	2.50	0.47
1:B:408:ASN:C	1:B:410:GLU:H	2.17	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:CD2	1:A:229:PHE:CE1	2.97	0.47
1:A:77:ALA:O	1:A:79:GLN:N	2.47	0.47
1:B:327:GLN:OE1	1:B:327:GLN:HA	2.14	0.47
1:B:149:LEU:C	1:B:149:LEU:CD2	2.83	0.47
1:B:99:LEU:HD11	1:B:112:GLN:HA	1.97	0.47
1:A:441:THR:HB	1:A:442:ARG:HD3	1.96	0.47
1:B:137:THR:C	1:B:139:LEU:N	2.68	0.47
1:B:277:TYR:CE1	1:B:294:ARG:HB3	2.50	0.47
1:B:371:ILE:HD12	1:B:475:VAL:HG23	1.97	0.47
1:B:508:ALA:CB	1:B:520:SER:HB3	2.43	0.47
1:A:180:ARG:HB2	1:A:251:MET:HE2	1.96	0.47
1:A:302:MET:CE	1:A:302:MET:HA	2.45	0.47
1:A:483:ASN:ND2	1:A:486:ALA:HB2	2.29	0.47
1:A:549:SER:HB3	1:B:117:ASN:HB3	1.96	0.47
1:B:525:PHE:CD1	1:B:525:PHE:C	2.88	0.46
1:B:363:LEU:O	1:B:366:ILE:HB	2.15	0.46
1:B:421:GLY:O	1:B:422:ASP:C	2.53	0.46
1:B:488:ASP:CB	1:B:491:GLN:HB2	2.44	0.46
1:A:211:LEU:O	1:A:212:ALA:HB3	2.14	0.46
1:A:277:TYR:CD2	1:A:312:VAL:HG21	2.51	0.46
1:A:83:VAL:HG13	1:A:84:PRO:HD2	1.97	0.46
1:A:182:LEU:HD23	1:A:182:LEU:O	2.15	0.46
1:B:486:ALA:HB2	1:B:492:ARG:NE	2.30	0.46
1:A:309:LEU:O	1:A:312:VAL:HG12	2.15	0.46
1:B:211:LEU:H	1:B:211:LEU:HD12	1.80	0.46
1:B:298:VAL:O	1:B:300:ALA:N	2.48	0.46
1:B:514:SER:O	1:B:515:ALA:HB3	2.16	0.46
1:B:529:ASP:O	1:B:530:TRP:CB	2.62	0.46
1:B:588:ILE:HG12	1:B:589:SER:N	2.30	0.46
1:A:401:GLY:HA3	1:A:462:PHE:CZ	2.51	0.46
1:B:241:LEU:HD21	1:B:248:ILE:HD11	1.97	0.46
1:B:277:TYR:CE2	1:B:312:VAL:HG21	2.51	0.46
1:A:77:ALA:C	1:A:79:GLN:H	2.19	0.46
1:A:77:ALA:C	1:A:79:GLN:N	2.69	0.46
1:B:241:LEU:CD2	1:B:241:LEU:C	2.84	0.46
1:B:368:ASN:O	1:B:369:CYS:O	2.34	0.46
1:B:370:THR:CG2	1:B:420:LEU:HD21	2.42	0.46
1:A:330:PHE:H	1:A:330:PHE:HD1	1.63	0.46
1:A:134:ILE:HD12	1:A:398:GLN:HG3	1.98	0.45
1:A:241:LEU:C	1:A:241:LEU:CD2	2.84	0.45
1:A:529:ASP:O	1:A:530:TRP:CB	2.65	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:HG3	1:B:278:TYR:CD1	2.50	0.45
1:A:279:ARG:NH2	2:A:2012:HOH:O	2.49	0.45
1:B:123:GLY:HA3	1:B:269:MET:O	2.15	0.45
1:A:93:ILE:O	1:A:95:ALA:N	2.44	0.45
1:B:241:LEU:HD23	1:B:242:PRO:HD2	1.97	0.45
1:B:535:TYR:HB3	1:B:550:ILE:CD1	2.46	0.45
1:A:309:LEU:C	1:A:312:VAL:HG12	2.36	0.45
1:B:408:ASN:C	1:B:410:GLU:N	2.70	0.45
1:A:199:ASN:OD1	1:A:201:TYR:HB2	2.17	0.45
1:A:355:THR:CG2	1:A:356:PRO:HD2	2.47	0.45
1:A:372:LEU:HD12	1:A:447:ILE:HD11	1.97	0.45
1:A:500:PHE:CE2	1:A:532:PRO:HG2	2.51	0.45
1:A:177:GLU:HG3	1:A:278:TYR:CD1	2.51	0.45
1:A:182:LEU:O	1:A:185:ILE:HB	2.16	0.45
1:B:149:LEU:HD22	1:B:168:LEU:HD11	1.97	0.45
1:B:229:PHE:CE2	1:B:348:ILE:HG23	2.51	0.45
1:B:545:ALA:C	1:B:547:LEU:H	2.19	0.45
1:A:455:THR:HG22	1:A:456:SER:N	2.31	0.45
1:A:202:LEU:CB	1:A:203:PRO:CD	2.95	0.45
1:A:381:THR:HG23	1:A:382:LEU:N	2.32	0.45
1:A:430:MET:O	1:A:432:PRO:HD3	2.17	0.45
1:A:443:LEU:HA	1:A:443:LEU:HD12	1.76	0.45
1:A:584:LEU:HG	1:A:585:LEU:HD12	1.97	0.45
1:B:141:GLY:O	1:B:144:MET:HB2	2.17	0.45
1:A:430:MET:HE2	1:B:265:VAL:H	1.79	0.45
1:B:443:LEU:HD12	1:B:443:LEU:HA	1.67	0.45
1:A:170:MET:CE	1:A:290:SER:HA	2.46	0.45
1:A:306:LEU:O	1:A:309:LEU:N	2.49	0.45
1:A:371:ILE:HD12	1:A:475:VAL:HG23	1.98	0.45
1:A:522:THR:C	1:A:524:ASP:H	2.20	0.45
1:A:551:LEU:HD21	1:B:479:LYS:HE3	1.98	0.45
1:B:148:GLN:NE2	1:B:581:SER:H	2.15	0.45
1:B:179:TYR:OH	1:B:236:ILE:HG23	2.16	0.45
1:A:241:LEU:HA	1:A:242:PRO:HD2	1.84	0.45
1:A:377:GLY:HA2	1:A:519:MET:CE	2.47	0.44
1:B:95:ALA:O	1:B:116:GLY:N	2.48	0.44
1:B:139:LEU:O	1:B:141:GLY:N	2.45	0.44
1:B:168:LEU:HA	1:B:329:MET:SD	2.57	0.44
1:B:195:TRP:CZ3	1:B:203:PRO:HG3	2.52	0.44
1:B:437:VAL:O	1:B:438:LEU:C	2.55	0.44
1:B:477:TYR:CE1	1:B:498:SER:HB2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ALA:HB1	1:B:467:CYS:HB3	1.99	0.44
1:B:99:LEU:CD1	1:B:112:GLN:HA	2.47	0.44
1:A:302:MET:HA	1:A:302:MET:HE2	1.99	0.44
1:A:70:TYR:OH	1:B:250:ARG:HD3	2.17	0.44
1:B:206:VAL:HG13	1:B:210:LEU:HD12	1.99	0.44
1:B:174:ALA:CB	1:B:320:ILE:HD12	2.45	0.44
1:B:359:ASP:CG	1:B:362:ILE:HG12	2.38	0.44
1:A:71:ALA:N	1:B:577:ALA:HB1	2.33	0.44
1:A:480:ASN:HD22	1:A:495:THR:HG23	1.82	0.44
1:B:296:TRP:HH2	1:B:312:VAL:HG11	1.82	0.44
1:A:122:MET:HB2	1:A:201:TYR:CD2	2.53	0.44
1:B:202:LEU:CB	1:B:203:PRO:CD	2.95	0.44
1:B:241:LEU:HD23	1:B:242:PRO:CD	2.48	0.44
1:A:228:GLN:HB3	1:A:310:PHE:CE2	2.53	0.44
1:A:190:THR:HG22	1:A:354:SER:N	2.33	0.44
1:A:244:TYR:C	1:A:244:TYR:CD1	2.91	0.44
1:A:420:LEU:N	1:A:420:LEU:HD23	2.23	0.44
1:B:357:VAL:HG12	1:B:358:PHE:N	2.33	0.44
1:A:428:HIS:HE1	1:A:555:ASP:OD2	2.01	0.43
1:A:479:LYS:HG3	1:A:479:LYS:O	2.17	0.43
1:A:549:SER:HB2	1:B:117:ASN:HB3	2.00	0.43
1:A:122:MET:HE3	1:A:210:LEU:HD22	1.99	0.43
1:A:372:LEU:HD12	1:A:447:ILE:CD1	2.49	0.43
1:B:224:ASN:HA	1:B:224:ASN:HD22	1.58	0.43
1:B:397:TRP:CD1	1:B:397:TRP:C	2.92	0.43
1:B:204:LYS:O	1:B:206:VAL:N	2.51	0.43
1:B:381:THR:CG2	1:B:382:LEU:N	2.77	0.43
1:B:476:LEU:HD12	1:B:476:LEU:N	2.34	0.43
1:B:213:ILE:HA	1:B:304:ARG:O	2.18	0.43
1:B:424:VAL:CG2	1:B:425:LEU:N	2.81	0.43
1:B:582:ALA:O	1:B:584:LEU:N	2.51	0.43
1:A:265:VAL:HG23	1:B:430:MET:CE	2.49	0.43
1:A:212:ALA:O	1:A:304:ARG:CG	2.66	0.43
1:A:397:TRP:C	1:A:397:TRP:CD1	2.91	0.43
1:A:525:PHE:C	1:A:525:PHE:CD1	2.92	0.43
1:A:446:THR:HG21	1:A:564:THR:HG22	2.00	0.43
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.78	0.43
1:A:361:ASP:O	1:A:365:GLN:HG3	2.19	0.43
1:A:168:LEU:CD2	1:A:168:LEU:C	2.88	0.43
1:A:128:TYR:OH	1:A:180:ARG:HD2	2.18	0.43
1:B:195:TRP:CH2	1:B:203:PRO:CB	3.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:O	1:A:254:VAL:HG23	2.19	0.42
1:A:187:ARG:NH2	1:A:272:PHE:O	2.52	0.42
1:A:262:SER:HA	1:A:358:PHE:CE1	2.53	0.42
1:A:566:VAL:O	1:A:569:ARG:HB2	2.19	0.42
1:A:442:ARG:NH2	1:B:70:TYR:CZ	2.86	0.42
1:A:428:HIS:HA	1:A:557:LYS:HD3	2.00	0.42
1:B:582:ALA:O	1:B:585:LEU:N	2.51	0.42
1:A:442:ARG:HG3	1:A:571:ASN:OD1	2.18	0.42
1:A:69:TRP:O	1:B:246:LYS:HD3	2.20	0.42
1:B:296:TRP:O	1:B:297:PRO:C	2.50	0.42
1:A:70:TYR:CZ	1:B:442:ARG:NH2	2.88	0.42
1:A:545:ALA:O	1:A:547:LEU:N	2.52	0.42
1:B:241:LEU:HA	1:B:242:PRO:HD2	1.88	0.42
1:B:445:ALA:HB2	1:B:467:CYS:CB	2.48	0.42
1:A:190:THR:HG22	1:A:354:SER:H	1.85	0.42
1:A:230:ASN:OD1	1:A:347:GLU:HB3	2.20	0.42
1:A:242:PRO:HG2	1:A:245:PHE:CE2	2.54	0.42
1:A:325:ASP:O	1:A:326:ALA:C	2.58	0.42
1:A:366:ILE:O	1:A:367:GLU:C	2.57	0.42
1:A:373:GLU:HG2	1:A:380:TRP:CG	2.54	0.42
1:B:236:ILE:HG22	1:B:237:ASN:N	2.35	0.42
1:B:545:ALA:O	1:B:547:LEU:N	2.53	0.42
1:A:505:VAL:HG22	1:A:537:THR:OG1	2.19	0.42
1:B:126:LEU:HD11	1:B:366:ILE:CD1	2.49	0.42
1:B:338:GLY:O	1:B:339:SER:C	2.58	0.42
1:A:562:ILE:HG22	1:A:566:VAL:HG11	2.00	0.42
1:B:280:TYR:HB2	1:B:320:ILE:CD1	2.50	0.42
1:B:505:VAL:HG12	1:B:506:THR:N	2.35	0.42
1:A:180:ARG:CZ	1:A:251:MET:HE2	2.50	0.42
1:A:442:ARG:NH1	1:A:442:ARG:CA	2.83	0.42
1:B:162:VAL:O	1:B:162:VAL:CG1	2.66	0.42
1:B:353:THR:O	1:B:353:THR:HG23	2.20	0.42
1:B:418:VAL:HG12	1:B:503:ILE:CD1	2.50	0.42
1:A:327:GLN:H	1:A:327:GLN:CD	2.24	0.42
1:A:526:THR:HB	1:B:554:GLY:H	1.85	0.42
1:B:296:TRP:HA	1:B:296:TRP:CE3	2.54	0.42
1:B:391:LYS:O	1:B:393:GLN:HG2	2.19	0.42
1:B:581:SER:O	1:B:582:ALA:C	2.57	0.42
1:A:489:ALA:O	1:A:492:ARG:HG3	2.20	0.41
1:B:154:ARG:HG2	1:B:154:ARG:NH1	2.35	0.41
1:A:445:ALA:HB1	1:A:467:CYS:HB3	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD23	1:A:475:VAL:HG13	2.02	0.41
1:B:329:MET:O	1:B:333:ILE:HG13	2.20	0.41
1:B:127:LEU:HD11	1:B:275:SER:HA	2.01	0.41
1:B:292:VAL:HA	1:B:386:ASN:OD1	2.20	0.41
1:A:114:PHE:CE2	1:B:548:ASN:HB2	2.55	0.41
1:B:554:GLY:O	1:B:556:LEU:N	2.53	0.41
1:B:77:ALA:C	1:B:79:GLN:N	2.73	0.41
1:A:480:ASN:HB3	1:A:495:THR:HG23	2.02	0.41
1:B:87:VAL:HG23	1:B:91:THR:OG1	2.21	0.41
1:B:104:SER:C	1:B:105:LEU:HD23	2.40	0.41
1:B:361:ASP:O	1:B:365:GLN:HG3	2.20	0.41
1:A:509:THR:C	1:A:511:ASP:H	2.23	0.41
1:B:133:GLY:O	1:B:134:ILE:C	2.59	0.41
1:B:171:THR:O	1:B:174:ALA:HB3	2.20	0.41
1:B:486:ALA:HB2	1:B:492:ARG:CZ	2.51	0.41
1:B:493:VAL:O	1:B:493:VAL:HG12	2.20	0.41
1:A:239:PHE:HA	1:A:330:PHE:CD2	2.55	0.41
1:A:292:VAL:HG12	1:A:293:TYR:N	2.35	0.41
1:A:391:LYS:HG2	1:A:391:LYS:H	1.62	0.41
1:A:381:THR:CG2	1:A:402:THR:HG23	2.48	0.41
1:B:391:LYS:O	1:B:393:GLN:N	2.54	0.41
1:B:442:ARG:NH1	1:B:442:ARG:HB2	2.32	0.41
1:A:554:GLY:H	1:B:526:THR:HB	1.86	0.41
1:A:102:ASP:HA	1:A:103:PRO:HD2	1.84	0.41
1:A:327:GLN:HA	1:A:330:PHE:CD1	2.56	0.41
1:B:380:TRP:CD1	1:B:380:TRP:N	2.89	0.41
1:A:445:ALA:CB	1:A:467:CYS:HB3	2.51	0.41
1:A:467:CYS:O	1:A:571:ASN:HB3	2.20	0.41
1:A:540:SER:HB2	1:A:546:ASN:O	2.21	0.41
1:B:401:GLY:HA3	1:B:462:PHE:CZ	2.56	0.41
1:B:447:ILE:N	1:B:447:ILE:HD12	2.29	0.41
1:A:247:SER:CA	1:A:578:LEU:HD22	2.36	0.41
1:B:202:LEU:O	1:B:203:PRO:O	2.39	0.41
1:A:557:LYS:CE	1:B:262:SER:HB2	2.36	0.41
1:A:330:PHE:O	1:A:333:ILE:HB	2.21	0.40
1:A:381:THR:HG21	1:A:402:THR:CG2	2.51	0.40
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.90	0.40
1:A:559:PRO:HD2	1:B:266:THR:HG21	2.03	0.40
1:B:397:TRP:CD1	1:B:397:TRP:O	2.74	0.40
1:B:539:THR:C	1:B:541:VAL:N	2.75	0.40
1:A:195:TRP:CD2	1:A:203:PRO:HB3	2.56	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:SER:H	1:A:548:ASN:HB3	1.85	0.40
1:A:584:LEU:HG	1:A:585:LEU:HD13	2.00	0.40
1:B:182:LEU:HD22	1:B:229:PHE:CE1	2.56	0.40
1:B:329:MET:O	1:B:330:PHE:C	2.59	0.40
1:A:187:ARG:NH1	1:A:187:ARG:CG	2.75	0.40
1:B:241:LEU:CD2	1:B:248:ILE:HD11	2.51	0.40
1:A:408:ASN:C	1:A:410:GLU:N	2.75	0.40
1:B:355:THR:CG2	1:B:356:PRO:HD2	2.51	0.40
1:B:355:THR:HG22	1:B:356:PRO:O	2.22	0.40
1:B:424:VAL:HG22	1:B:425:LEU:H	1.86	0.40
1:B:582:ALA:O	1:B:585:LEU:HB2	2.22	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	523/525 (100%)	408 (78%)	84 (16%)	31 (6%)	2	17
1	B	523/525 (100%)	414 (79%)	74 (14%)	35 (7%)	1	14
All	All	1046/1050 (100%)	822 (79%)	158 (15%)	66 (6%)	1	16

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	202	LEU
1	A	203	PRO
1	A	205	GLN
1	A	326	ALA
1	A	369	CYS
1	A	442	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	487	GLU
1	A	513	THR
1	B	110	LYS
1	B	202	LEU
1	B	205	GLN
1	B	240	ALA
1	B	369	CYS
1	B	392	GLY
1	B	442	ARG
1	B	513	THR
1	B	582	ALA
1	A	89	ALA
1	A	94	LYS
1	A	107	SER
1	A	134	ILE
1	A	141	GLY
1	A	160	ALA
1	A	284	THR
1	A	409	THR
1	A	443	LEU
1	A	516	TYR
1	A	523	LEU
1	A	525	PHE
1	B	76	VAL
1	B	107	SER
1	B	108	GLY
1	B	140	ASP
1	B	155	LYS
1	B	203	PRO
1	B	299	GLY
1	B	443	LEU
1	B	523	LEU
1	B	546	ASN
1	B	555	ASP
1	B	583	ASN
1	A	78	LYS
1	A	82	ASN
1	A	546	ASN
1	A	555	ASP
1	B	117	ASN
1	B	204	LYS
1	B	393	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	441	THR
1	B	530	TRP
1	A	72	PRO
1	A	88	LEU
1	A	245	PHE
1	A	250	ARG
1	A	304	ARG
1	B	161	LYS
1	B	347	GLU
1	A	240	ALA
1	B	86	ASN
1	B	134	ILE
1	B	352	GLU
1	B	382	LEU
1	B	303	PRO
1	B	460	VAL
1	B	493	VAL

### 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	449/449 (100%)	410 (91%)	39 (9%)	12	43
1	B	449/449 (100%)	413 (92%)	36 (8%)	14	48
All	All	898/898 (100%)	823 (92%)	75 (8%)	13	45

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

Mol	Chain	Res	Type
1	A	70	TYR
1	A	97	VAL
1	A	101	TYR
1	A	154	ARG
1	A	163	TYR
1	A	187	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	190	THR
1	A	210	LEU
1	A	225	TYR
1	A	241	LEU
1	A	251	MET
1	A	256	SER
1	A	259	PHE
1	A	268	GLN
1	A	279	ARG
1	A	280	TYR
1	A	295	ASP
1	A	296	TRP
1	A	316	LEU
1	A	328	THR
1	A	381	THR
1	A	388	THR
1	A	390	SER
1	A	397	TRP
1	A	404	THR
1	A	439	GLU
1	A	442	ARG
1	A	461	THR
1	A	478	PHE
1	A	480	ASN
1	A	484	ASP
1	A	488	ASP
1	A	495	THR
1	A	510	ASP
1	A	526	THR
1	A	550	ILE
1	A	562	ILE
1	A	563	THR
1	A	564	THR
1	B	70	TYR
1	B	117	ASN
1	B	140	ASP
1	B	154	ARG
1	B	163	TYR
1	B	164	GLU
1	B	167	ASP
1	B	168	LEU
1	B	173	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	182	LEU
1	B	224	ASN
1	B	236	ILE
1	B	241	LEU
1	B	251	MET
1	B	268	GLN
1	B	283	THR
1	B	287	SER
1	B	295	ASP
1	B	296	TRP
1	B	316	LEU
1	B	387	VAL
1	B	388	THR
1	B	389	GLN
1	B	397	TRP
1	B	439	GLU
1	B	442	ARG
1	B	447	ILE
1	B	457	SER
1	B	461	THR
1	B	465	THR
1	B	478	PHE
1	B	526	THR
1	B	550	ILE
1	B	562	ILE
1	B	584	LEU
1	B	585	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	193	ASN
1	A	205	GLN
1	A	393	GLN
1	A	398	GLN
1	A	480	ASN
1	A	483	ASN
1	B	148	GLN
1	B	176	GLN
1	B	193	ASN
1	B	224	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	228	GLN
1	B	389	GLN
1	B	398	GLN
1	B	543	ASN
1	B	583	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	525/525 (100%)	0.40	19 (3%)	43	39	16, 31, 60, 85	0
1	B	525/525 (100%)	0.45	23 (4%)	35	32	14, 31, 62, 103	0
All	All	1050/1050 (100%)	0.43	42 (4%)	39	35	14, 31, 62, 103	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	ASP	5.4
1	A	299	GLY	4.4
1	A	287	SER	4.3
1	B	107	SER	3.6
1	B	105	LEU	3.5
1	B	86	ASN	3.4
1	A	386	ASN	3.2
1	A	515	ALA	3.2
1	B	282	ALA	3.2
1	B	299	GLY	3.1
1	B	289	THR	3.0
1	B	590	THR	3.0
1	A	452	ALA	2.9
1	A	514	SER	2.8
1	B	586	SER	2.8
1	B	488	ASP	2.7
1	B	201	TYR	2.7
1	B	589	SER	2.7
1	A	240	ALA	2.7
1	B	157	ASN	2.6
1	A	417	ALA	2.6
1	B	164	GLU	2.5
1	A	209	GLN	2.5
1	A	292	VAL	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	74	GLU	2.4
1	B	287	SER	2.3
1	B	108	GLY	2.3
1	B	541	VAL	2.3
1	A	376	ALA	2.3
1	B	587	ASN	2.3
1	B	340	ASP	2.2
1	A	300	ALA	2.2
1	B	483	ASN	2.2
1	B	512	PRO	2.2
1	B	452	ALA	2.2
1	A	513	THR	2.2
1	B	111	ASP	2.0
1	A	456	SER	2.0
1	A	283	THR	2.0
1	A	234	GLN	2.0
1	A	589	SER	2.0
1	A	157	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.