



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:50 PM UTC

PDB ID : 2VF1 / pdb_00002vf1
Title : X-ray crystallographic structure of the picobirnavirus 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

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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

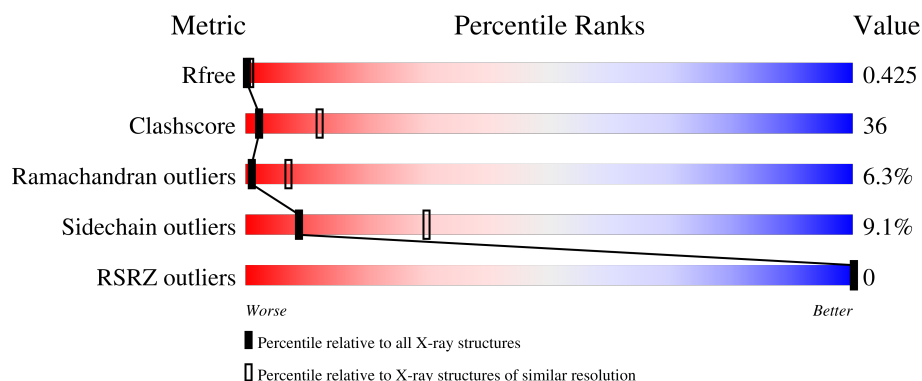
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

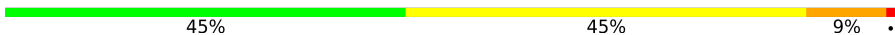
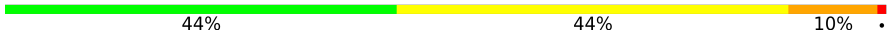
The reported resolution of this entry is 3.40 Å.

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))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 ≥ 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 $\leq 5\%$. 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	
1	B	525	

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

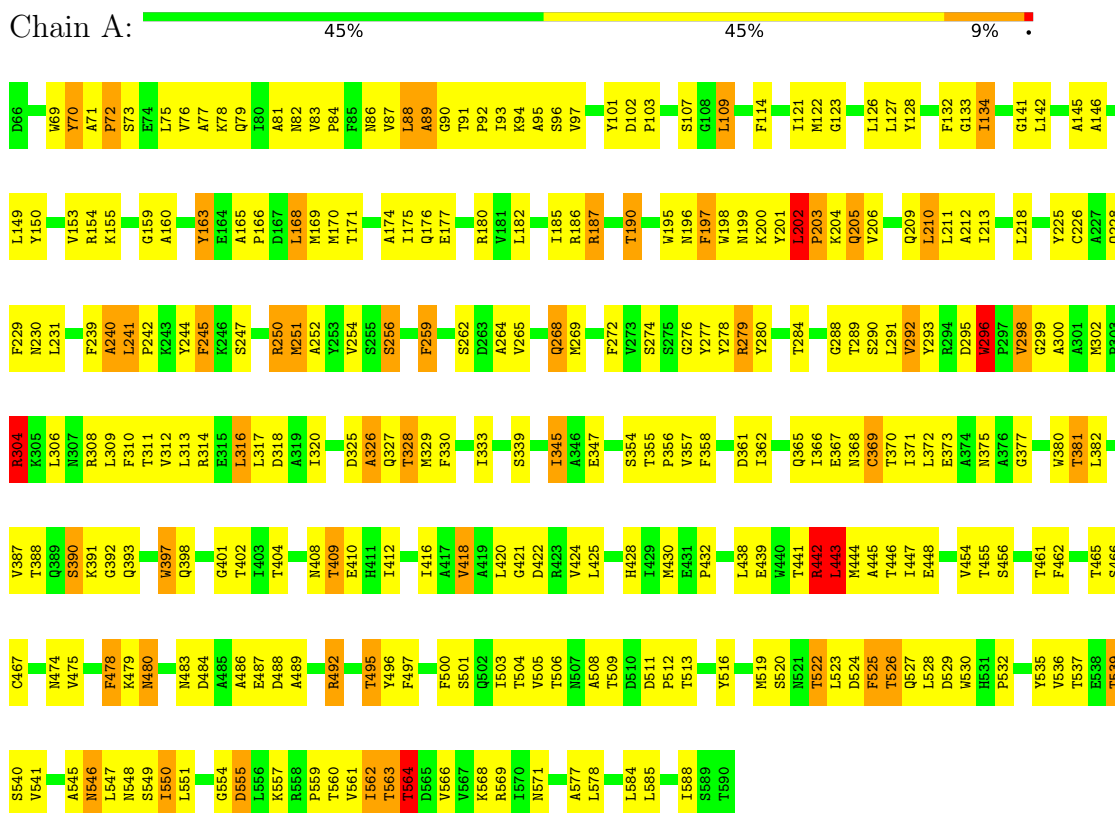
- Molecule 2 is water.

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

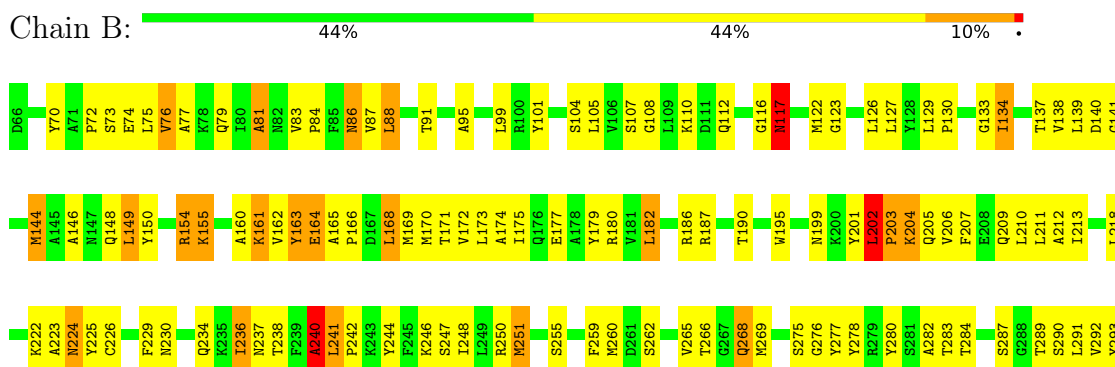
3 Residue-property plots

These plots are drawn for all protein, RNA, 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 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



T526	T533	T539	T540	V541	N542	V544	A545	N546	L547	N548	S549	T550	G554	D555	L556	K557	R558	P559	T560	V561	I562	T563	T564	K568	R569	I570	N571	S572	A577	L578	S581	A582	N583	L584	L585	S586	N587	I588	S589	T590												
T446	S457	T465	T466	S466	C467	E470	L471	V475	L476	Y477	F478	K479	W482	A486	E487	D488	Q491	R492	V493	F497	S498	Q502	I503	T504	V505	T506	R507	A508	T509	D510	D511	P512	T513	S514	A515	M519	S520	L523	D524	F525												
E367	N368	C369	T370	I371	L372	E373	A374	N375	W380	T381	L382	N386	V387	T388	Q389	K390	K391	G392	Q393	V394	L395	L396	W397	G401	N408	T409	E410	H411	I412	I416	A417	V418	A419	L420	G421	D422	R423	V424	L425	M430	Y434	S435	D436	V437	L438	E439	W440	T441	R442	L443	M444	A445
R294	D295	V296	P297	V298	Q299	A300	A301	M302	P303	R304	K305	L306	N307	R308	L309	V312	L316	I320	D323	A324	D325	A326	Q327	T328	M329	F330	I333	G338	S339	T340	G341	S344	E347	I348	D351	E352	T353	S354	T355	P356	V357	F358	D359	V360	D361	I362	L363	A364	Q365	I366		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	407.42Å 407.42Å 808.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.98 – 3.40 49.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	70.0 (49.98-3.40) 43.5 (49.98-3.40)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.273 , 0.272 0.425 , 0.425	Depositor DCC
R_{free} test set	23009 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.087 for -h,-k,l	Xtriage
F_o, F_c correlation	0.19	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.55	0/4209	1.06	21/5737 (0.4%)
1	B	0.57	1/4209 (0.0%)	1.08	21/5737 (0.4%)
All	All	0.56	1/8418 (0.0%)	1.07	42/11474 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	587	ASN	CA-C	5.28	1.58	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	TRP	CA-C-N	-11.14	105.91	119.84
1	A	296	TRP	C-N-CA	-11.14	105.91	119.84
1	B	296	TRP	CA-C-N	-10.17	107.13	119.84
1	B	296	TRP	C-N-CA	-10.17	107.13	119.84
1	B	304	ARG	N-CA-C	8.87	121.77	110.24
1	A	454	VAL	N-CA-C	7.09	119.16	108.80
1	A	564	THR	N-CA-C	-7.02	103.63	111.28
1	A	296	TRP	N-CA-C	-6.88	99.24	109.42
1	B	284	THR	N-CA-C	6.80	120.46	111.75
1	A	443	LEU	N-CA-C	-6.75	96.41	110.80
1	B	443	LEU	N-CA-C	-6.65	96.64	110.80
1	A	298	VAL	N-CA-C	6.61	123.09	109.34
1	A	186	ARG	N-CA-C	-6.60	103.78	110.97
1	B	520	SER	N-CA-C	-6.55	100.28	110.17
1	B	454	VAL	N-CA-C	6.40	118.36	108.44
1	A	202	LEU	N-CA-C	6.12	123.33	109.81
1	A	492	ARG	N-CA-C	-6.10	105.84	113.28
1	B	341	GLY	N-CA-C	-6.08	105.22	115.62
1	B	240	ALA	N-CA-C	6.04	123.66	110.80
1	B	298	VAL	N-CA-C	5.98	121.79	109.34
1	B	416	ILE	N-CA-C	5.87	116.32	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	GLN	N-CA-C	5.86	120.00	112.86
1	B	418	VAL	N-CA-C	5.73	116.94	108.45
1	A	318	ASP	N-CA-C	-5.70	105.16	111.71
1	B	296	TRP	N-CA-C	-5.61	99.29	109.44
1	A	96	SER	N-CA-C	5.57	118.63	109.72
1	B	487	GLU	N-CA-C	-5.57	105.75	112.54
1	B	202	LEU	N-CA-C	5.50	121.97	109.81
1	A	339	SER	N-CA-C	-5.44	105.46	111.71
1	A	304	ARG	N-CA-C	5.37	122.23	110.80
1	B	412	ILE	N-CA-C	-5.35	107.16	113.42
1	A	561	VAL	N-CA-C	5.32	116.25	108.53
1	B	588	ILE	N-CA-C	5.28	117.16	108.97
1	A	416	ILE	N-CA-C	5.20	115.34	107.75
1	A	412	ILE	N-CA-C	-5.17	107.79	112.96
1	B	459	LYS	N-CA-C	5.14	120.95	114.31
1	A	90	GLY	N-CA-C	5.13	120.31	114.67
1	B	81	ALA	N-CA-C	-5.08	107.63	113.88
1	B	584	LEU	N-CA-C	-5.08	105.40	112.30
1	B	523	LEU	N-CA-C	5.07	121.59	110.80
1	A	292	VAL	N-CA-C	5.04	116.51	109.55
1	A	522	THR	N-CA-C	-5.02	102.47	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	299	0
1	B	4117	0	4038	334	0
2	A	22	0	0	2	0
2	B	30	0	0	0	0
All	All	8286	0	8076	595	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 36.

All (595) 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:HG2	1:A:187:ARG:HH11	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:N	1:B:442:ARG:HH11	1.61	0.96
1:A:174:ALA:HB1	1:A:320:ILE:HD12	1.47	0.95
1:B:146:ALA:HA	1:B:169:MET:HE2	1.48	0.93
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:HD12	1:B:88:LEU:H	1.38	0.89
1:A:377:GLY:HA2	1:A:519:MET:HE3	1.54	0.89
1:A:122:MET:HE3	1:A:210:LEU:HD22	1.55	0.88
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:HB2	1:B:442:ARG:CZ	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:A:122:MET:HE1	1:A:209:GLN:HB2	1.59	0.84
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:A:268:GLN:CD	1:A:268:GLN:H	1.82	0.83
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:N	1:A:163:TYR:HD2	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:B:268:GLN:H	1:B:268:GLN:CD	1.89	0.80
1:B:122:MET:HE1	1:B:209:GLN:HB2	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:202:LEU:O	1:A:203:PRO:C	2.28	0.76
1:A:175:ILE:HD13	1:A:239:PHE:HB3	1.67	0.76
1:B:302:MET:HE2	1:B:303:PRO:HD2	1.68	0.75
1:B:441:THR:HG22	1:B:442:ARG:N	2.01	0.74
1:A:170:MET:HE3	1:A:290:SER:HA	1.70	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:HG2	1:A:187:ARG:NH1	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:B:180:ARG:N	1:B:251:MET:HE1	2.03	0.73
1:B:202:LEU:O	1:B:203:PRO:C	2.30	0.73
1:A:430:MET:CE	1:B:265:VAL:H	2.02	0.73
1:A:265:VAL:H	1:B:430:MET:HE2	1.54	0.72
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:A:302:MET:HE2	1:A:302:MET:HA	1.71	0.72
1:B:187:ARG:HD3	1:B:211:LEU:CD2	2.18	0.72
1:A:146:ALA:HB2	1:A:169:MET:HG2	1.72	0.72
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:N	1:B:442:ARG:NH1	2.39	0.71
1:B:447:ILE:HD12	1:B:447:ILE:H	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:HD12	1:B:88:LEU:N	2.07	0.69
1:A:375:ASN:HA	1:A:501:SER:HB3	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:89:ALA:CB	1:A:199:ASN:HA	2.26	0.66
1:A:239:PHE:HA	1:A:330:PHE:CE2	2.31	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:B:225:TYR:CE1	1:B:306:LEU:HB2	2.32	0.65
1:B:276:GLY:HA3	1:B:293:TYR:CE1	2.33	0.64
1:B:73:SER:HB3	1:B:76:VAL:CG1	2.25	0.64
1:B:163:TYR:N	1:B:163:TYR:CD2	2.66	0.64
1:A:430:MET:HE2	1:B:265:VAL:H	1.62	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:HD23	1:B:420:LEU:H	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:87:VAL:HG13	1:A:87:VAL:O	1.97	0.63
1:A:441:THR:HG22	1:A:442:ARG:N	2.14	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:557:LYS:HE3	1:B:262:SER:CB	2.29	0.62
1:B:162:VAL:HG12	1:B:162:VAL:O	2.00	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
1:A:508:ALA:HB3	1:A:520:SER:HB3	1.81	0.61
1:B:162:VAL:C	1:B:163:TYR:HD2	2.08	0.61
1:A:88:LEU:CD1	1:A:200:LYS:HE3	2.31	0.61
1:B:99:LEU:O	1:B:99:LEU:HD12	2.00	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:A:180:ARG:HB2	1:A:251:MET:HE1	1.82	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:N	1:A:259:PHE:CD1	2.69	0.60
1:A:146:ALA:HA	1:A:169:MET:HE2	1.83	0.60
1:B:268:GLN:CD	1:B:268:GLN:N	2.59	0.60
1:A:168:LEU:HD23	1:A:168:LEU:C	2.27	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:88:LEU:H	1:B:88:LEU:CD1	2.13	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:326:ALA:O	1:B:329:MET:HB2	2.02	0.58
1:B:582:ALA:C	1:B:584:LEU:H	2.12	0.58
1:B:149:LEU:C	1:B:149:LEU:HD23	2.29	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:84:PRO:HB2	1:A:86:ASN:ND2	2.20	0.56
1:B:179:TYR:CZ	1:B:236:ILE:HG23	2.40	0.56
1:A:278:TYR:O	1:A:316:LEU:HD21	2.05	0.56
1:A:239:PHE:HA	1:A:330:PHE:HE2	1.71	0.56
1:A:277:TYR:O	1:A:293:TYR:HD1	1.87	0.56
1:B:163:TYR:CE1	1:B:329:MET:HG2	2.40	0.56
1:A:149:LEU:C	1:A:149:LEU:HD13	2.30	0.56
1:B:460:VAL:HG12	1:B:460:VAL:O	2.05	0.56
1:A:72:PRO:HG2	1:A:73:SER:H	1.69	0.56
1:A:478:PHE:CD1	1:A:478:PHE:N	2.74	0.56
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: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:B:122:MET:HE3	1:B:210:LEU:HG	1.87	0.55
1:B:174:ALA:HB1	1:B:320:ILE:CD1	2.36	0.55
1:B:302:MET:HE2	1:B:302:MET:HA	1.87	0.55
1:A:196:ASN:O	1:A:198:TRP:N	2.39	0.55
1:A:408:ASN:C	1:A:410:GLU:H	2.15	0.55
1:B:478:PHE:CD1	1:B:478:PHE:N	2.74	0.55
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.89	0.55
1:B:137:THR:C	1:B:139:LEU:H	2.14	0.55
1:B:259:PHE:N	1:B:259:PHE:CD1	2.75	0.55
1:A:274:SER:O	1:A:296:TRP:HD1	1.90	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:A:424:VAL:HG22	1:A:425:LEU:N	2.22	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:CZ	1:B:442:ARG:CB	2.83	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLY:HA2	1:A:564:THR:HG23	1.89	0.54
1:A:171:THR:OG1	1:A:329:MET:HE1	2.07	0.54
1:B:146:ALA:CA	1:B:169:MET:HE2	2.29	0.54
1:A:127:LEU:HD23	1:A:474:ASN:HD21	1.73	0.54
1:A:251:MET:HG3	1:A:252:ALA:N	2.23	0.54
1:A:409:THR:HG22	1:A:409:THR:O	2.06	0.53
1:A:430:MET:HE1	1:B:265:VAL:H	1.73	0.53
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:302:MET:CE	1:B:303:PRO:HD2	2.36	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
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:212:ALA:C	1:A:213:ILE:HD13	2.33	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:O	1:B:348:ILE:HG13	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:176:GLN:HG2	1:A:251:MET:HE3	1.90	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:HD23	1:A:109:LEU:N	2.24	0.52
1:A:196:ASN:O	1:A:197:PHE:C	2.51	0.52
1:A:365:GLN:C	1:A:443:LEU:HD23	2.35	0.52
1:B:370:THR:HB	1:B:445:ALA:H	1.74	0.52
1:B:408:ASN:C	1:B:410:GLU:H	2.17	0.52
1:B:190:THR:HG22	1:B:354:SER:N	2.25	0.52
1:A:133:GLY:O	1:A:134:ILE:C	2.52	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:A:545:ALA:C	1:A:547:LEU:H	2.18	0.52
1:B:149:LEU:C	1:B:149:LEU:CD2	2.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HG22	1:B:138:VAL:N	2.25	0.52
1:A:420:LEU:H	1:A:420:LEU:CD2	2.21	0.51
1:B:72:PRO:HG2	1:B:76:VAL:CG1	2.23	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:B:525:PHE:CD1	1:B:525:PHE:C	2.88	0.51
1:B:130:PRO:HB2	1:B:278:TYR:HE1	1.75	0.51
1:B:421:GLY:O	1:B:422:ASP:C	2.53	0.51
1:B:81:ALA:O	1:B:83:VAL:N	2.44	0.51
1:B:234:GLN:O	1:B:238:THR:HG23	2.10	0.51
1:B:122:MET:HB2	1:B:201:TYR:CD2	2.45	0.51
1:B:241:LEU:C	1:B:241:LEU:CD2	2.84	0.51
1:B:371:ILE:HD12	1:B:475:VAL:CG2	2.41	0.51
1:B:442:ARG:H	1:B:442:ARG:CD	2.21	0.51
1:B:470:GLU:O	1:B:471:LEU:HB3	2.10	0.51
1:B:199:ASN:OD1	1:B:201:TYR:HB2	2.11	0.51
1:A:77:ALA:C	1:A:79:GLN:H	2.19	0.50
1:B:75:LEU:O	1:B:77:ALA:N	2.44	0.50
1:B:154:ARG:HG2	1:B:154:ARG:HH11	1.76	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:296:TRP:O	1:B:297:PRO:C	2.50	0.50
1:A:73:SER:OG	1:A:76:VAL:HG23	2.11	0.50
1:A:226:CYS:O	1:A:229:PHE:HB3	2.12	0.50
1:A:241:LEU:C	1:A:241:LEU:CD2	2.84	0.50
1:B:187:ARG:NH2	1:B:255:SER:HA	2.26	0.50
1:A:442:ARG:CZ	1:A:442:ARG:CB	2.86	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: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:HH11	1:B:442:ARG:H	1.52	0.50
1:A:309:LEU:C	1:A:312:VAL:HG12	2.36	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:H	1:A:442:ARG:CD	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ALA:C	1:B:547:LEU:H	2.19	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:148:GLN:NE2	1:B:582:ALA:H	2.00	0.49
1:B:280:TYR:HB2	1:B:320:ILE:HD13	1.94	0.49
1:B:260:MET:HE2	1:B:356:PRO:O	2.12	0.49
1:A:175:ILE:CD1	1:A:239:PHE:HB3	2.39	0.49
1:A:522:THR:C	1:A:524:ASP:H	2.20	0.49
1:B:424:VAL:HG11	1:B:533:ILE:HG21	1.93	0.49
1:A:163:TYR:CD1	1:A:329:MET:HG2	2.47	0.49
1:A:279:ARG:O	1:A:291:LEU:HD12	2.12	0.49
1:B:186:ARG:HD2	1:B:229:PHE:CZ	2.48	0.49
1:B:442:ARG:NH1	1:B:442:ARG:CA	2.75	0.49
1:B:437:VAL:O	1:B:438:LEU:C	2.55	0.49
1:A:149:LEU:O	1:A:153:VAL:HG23	2.12	0.49
1:B:218:LEU:O	1:B:218:LEU:HD12	2.13	0.49
1:A:122:MET:CE	1:A:210:LEU:HD22	2.37	0.49
1:B:144:MET:HA	1:B:144:MET:HE2	1.94	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:359:ASP:CG	1:B:362:ILE:HG12	2.38	0.49
1:B:540:SER:H	1:B:548:ASN:HB3	1.77	0.49
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:121:ILE:HG23	1:A:478:PHE:O	2.13	0.48
1:A:422:ASP:OD1	1:A:563:THR:HA	2.12	0.48
1:A:268:GLN:CD	1:A:268:GLN:N	2.59	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:77:ALA:C	1:A:79:GLN:N	2.69	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:A:244:TYR:CD1	1:A:244:TYR:C	2.91	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:O	1:B:251:MET:HG3	2.13	0.48
1:A:277:TYR:CE2	1:A:312:VAL:HG21	2.49	0.48
1:B:397:TRP:CD1	1:B:397:TRP:C	2.92	0.48
1:A:91:THR:HB	1:A:92:PRO:HD2	1.95	0.48
1:A:296:TRP:CE3	1:A:296:TRP:HA	2.48	0.48
1:A:505:VAL:HG12	1:A:506:THR:N	2.28	0.48
1:B:137:THR:C	1:B:139:LEU:N	2.68	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:89:ALA:HB3	1:A:199:ASN:HA	1.96	0.47
1:A:155:LYS:HE3	1:A:588:ILE:HG23	1.95	0.47
1:A:316:LEU:O	1:A:320:ILE:HG12	2.14	0.47
1:A:397:TRP:CD1	1:A:397:TRP:C	2.91	0.47
1:A:525:PHE:CD1	1:A:525:PHE:C	2.92	0.47
1:B:84:PRO:CG	1:B:86:ASN:ND2	2.77	0.47
1:A:441:THR:O	1:A:443:LEU:N	2.47	0.47
1:B:162:VAL:C	1:B:163:TYR:CD2	2.91	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:B:212:ALA:O	1:B:304:ARG:HG2	2.14	0.47
1:A:522:THR:O	1:A:524:ASP:N	2.48	0.47
1:A:168:LEU:C	1:A:168:LEU:CD2	2.88	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:A:77:ALA:O	1:A:79:GLN:N	2.47	0.47
1:A:180:ARG:CZ	1:A:251:MET:HE2	2.44	0.47
1:A:182:LEU:CD2	1:A:229:PHE:CE1	2.97	0.47
1:B:327:GLN:OE1	1:B:327:GLN:HA	2.14	0.47
1:A:366:ILE:O	1:A:367:GLU:C	2.57	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: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:A:146:ALA:CA	1:A:169:MET:HE2	2.45	0.47
1:B:338:GLY:O	1:B:339:SER:C	2.58	0.47
1:B:508:ALA:CB	1:B:520:SER:HB3	2.43	0.47
1:A:325:ASP:O	1:A:326:ALA:C	2.58	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:A:327:GLN:CD	1:A:327:GLN:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:MET:HE2	1:B:478:PHE:HB2	1.96	0.46
1:B:363:LEU:O	1:B:366:ILE:HB	2.15	0.46
1:B:488:ASP:CB	1:B:491:GLN:HB2	2.44	0.46
1:B:581:SER:O	1:B:582:ALA:C	2.57	0.46
1:A:83:VAL:HG13	1:A:84:PRO:HD2	1.97	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: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:77:ALA:C	1:B:79:GLN:N	2.73	0.46
1:B:211:LEU:HD12	1:B:211:LEU:H	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:B:104:SER:C	1:B:105:LEU:HD23	2.40	0.46
1:B:133:GLY:O	1:B:134:ILE:C	2.59	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:529:ASP:O	1:A:530:TRP:CB	2.65	0.45
1:B:170:MET:HE3	1:B:290:SER:HA	1.97	0.45
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:509:THR:C	1:A:511:ASP:H	2.23	0.45
1:B:539:THR:C	1:B:541:VAL:N	2.75	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:B:329:MET:O	1:B:330:PHE:C	2.59	0.45
1:B:408:ASN:C	1:B:410:GLU:N	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:302:MET:HA	1:A:302:MET:CE	2.45	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:A:408:ASN:C	1:A:410:GLU:N	2.75	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:HD12	1:A:443:LEU:HA	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:B:443:LEU:HD12	1:B:443:LEU:HA	1.67	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: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:155:LYS:HZ3	1:B:588:ILE:HB	1.82	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:B:497:PHE:CD1	1:B:497:PHE:C	2.94	0.45
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:477:TYR:CE1	1:B:498:SER:HB2	2.52	0.44
1:B:351:ASP:O	1:B:352:GLU:C	2.59	0.44
1:B:99:LEU:CD1	1:B:112:GLN:HA	2.47	0.44
1:B:445:ALA:HB1	1:B:467:CYS:HB3	1.99	0.44
1:A:70:TYR:OH	1:B:250:ARG:HD3	2.17	0.44
1:A:71:ALA:N	1:B:577:ALA:HB1	2.33	0.44
1:B:174:ALA:CB	1:B:320:ILE:HD12	2.45	0.44
1:B:206:VAL:HG13	1:B:210:LEU:HD12	1.99	0.44
1:A:390:SER:C	1:A:392:GLY:N	2.74	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:A:455:THR:HG22	1:A:456:SER:N	2.31	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:B:511:ASP:O	1:B:512:PRO:C	2.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420:LEU:HD23	1:A:420:LEU:N	2.23	0.44
1:B:357:VAL:HG12	1:B:358:PHE:N	2.33	0.44
1:B:170:MET:HE3	1:B:289:THR:O	2.17	0.43
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:372:LEU:HD12	1:A:447:ILE:CD1	2.49	0.43
1:A:539:THR:C	1:A:541:VAL:N	2.75	0.43
1:B:224:ASN:HD22	1:B:224:ASN:HA	1.58	0.43
1:B:160:ALA:O	1:B:161:LYS:C	2.61	0.43
1:B:222:LYS:O	1:B:223:ALA:C	2.61	0.43
1:A:145:ALA:HB3	1:A:169:MET:HE3	2.00	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:571:ASN:O	1:B:572:SER:C	2.61	0.43
1:B:77:ALA:C	1:B:79:GLN:H	2.27	0.43
1:B:306:LEU:O	1:B:307:ASN:C	2.60	0.43
1:A:522:THR:C	1:A:524:ASP:N	2.77	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:212:ALA:O	1:A:304:ARG:CG	2.66	0.43
1:A:265:VAL:HG23	1:B:430:MET:CE	2.49	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: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
1:A:187:ARG:NH2	1:A:272:PHE:O	2.52	0.42
1:A:250:ARG:O	1:A:254:VAL:HG23	2.19	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:428:HIS:HA	1:A:557:LYS:HD3	2.00	0.42
1:A:442:ARG:NH2	1:B:70:TYR:CZ	2.86	0.42
1:B:366:ILE:O	1:B:367:GLU:C	2.62	0.42
1:B:582:ALA:O	1:B:585:LEU:N	2.51	0.42
1:A:69:TRP:O	1:B:246:LYS:HD3	2.20	0.42
1:A:70:TYR:CZ	1:B:442:ARG:NH2	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TYR:CD1	1:A:101:TYR:C	2.98	0.42
1:A:262:SER:C	1:A:264:ALA:H	2.27	0.42
1:A:442:ARG:HG3	1:A:571:ASN:OD1	2.18	0.42
1:A:250:ARG:O	1:A:251:MET:C	2.63	0.42
1:A:545:ALA:C	1:A:547:LEU:N	2.76	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:B:563:THR:O	1:B:564:THR:C	2.62	0.42
1:B:582:ALA:C	1:B:584:LEU:N	2.76	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:368:ASN:O	1:A:444:MET:HE2	2.20	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:310:PHE:C	1:A:312:VAL:N	2.77	0.42
1:A:505:VAL:HG22	1:A:537:THR:OG1	2.19	0.42
1:B:101:TYR:CD1	1:B:101:TYR:C	2.98	0.42
1:B:126:LEU:HD11	1:B:366:ILE:CD1	2.49	0.42
1:B:368:ASN:HB3	1:B:444:MET:HE3	2.01	0.42
1:B:434:TYR:CD1	1:B:434:TYR:C	2.98	0.42
1:A:170:MET:HE3	1:A:290:SER:CA	2.44	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:442:ARG:NH1	1:A:442:ARG:CA	2.83	0.42
1:B:75:LEU:C	1:B:77:ALA:N	2.77	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:526:THR:HB	1:B:554:GLY:H	1.85	0.42
1:B:73:SER:O	1:B:74:GLU:C	2.62	0.42
1:B:75:LEU:O	1:B:76:VAL:C	2.63	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:438:LEU:C	1:B:438:LEU:HD23	2.45	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:B:168:LEU:C	1:B:168:LEU:CD2	2.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ASP:O	1:B:519:MET:HE3	2.20	0.41
1:B:584:LEU:C	1:B:584:LEU:HD12	2.45	0.41
1:A:126:LEU:HD23	1:A:475:VAL:HG13	2.02	0.41
1:A:265:VAL:H	1:B:430:MET:HE1	1.82	0.41
1:A:368:ASN:HB3	1:A:444:MET:HE3	2.02	0.41
1:A:445:ALA:HB1	1:A:467:CYS:HB3	2.01	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:A:497:PHE:CD1	1:A:497:PHE:C	2.98	0.41
1:B:554:GLY:O	1:B:556:LEU:N	2.53	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:180:ARG:CA	1:B:251:MET:HE1	2.50	0.41
1:B:326:ALA:HA	1:B:329:MET:HE3	2.01	0.41
1:B:361:ASP:O	1:B:365:GLN:HG3	2.20	0.41
1:A:241:LEU:C	1:A:241:LEU:HD23	2.45	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:B:509:THR:C	1:B:511:ASP:H	2.28	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:381:THR:CG2	1:A:402:THR:HG23	2.48	0.41
1:A:391:LYS:H	1:A:391:LYS:HG2	1.62	0.41
1:A:511:ASP:O	1:A:512:PRO:C	2.63	0.41
1:A:554:GLY:H	1:B:526:THR:HB	1.86	0.41
1:B:391:LYS:O	1:B:393:GLN:N	2.54	0.41
1:B:442:ARG:HB2	1:B:442:ARG:NH1	2.32	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: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:368:ASN:O	1:B:444:MET:HE2	2.20	0.41
1:B:380:TRP:N	1:B:380:TRP:CD1	2.89	0.41
1:B:401:GLY:HA3	1:B:462:PHE:CZ	2.56	0.41
1:B:447:ILE:HD12	1:B:447:ILE:N	2.29	0.41
1:B:584:LEU:C	1:B:584:LEU:CD1	2.94	0.41
1:A:247:SER:CA	1:A:578:LEU:HD22	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:559:PRO:HD2	1:B:266:THR:HG21	2.03	0.40
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.90	0.40
1:B:397:TRP:CD1	1:B:397:TRP:O	2.74	0.40
1:A:195:TRP:CD2	1:A:203:PRO:HB3	2.56	0.40
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: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:B:365:GLN:C	1:B:443:LEU:HD23	2.46	0.40
1:A:75:LEU:HD23	1:A:75:LEU:C	2.47	0.40
1:A:306:LEU:C	1:A:308:ARG:N	2.79	0.40
1:B:355:THR:CG2	1:B:356:PRO:HD2	2.51	0.40
1:A:288:GLY:O	1:A:289:THR:C	2.64	0.40
1:B:226:CYS:HG	1:B:348:ILE:HD11	1.82	0.40
1:B:323:ASP:O	1:B:324:ALA:C	2.64	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%)	1	8
1	B	523/525 (100%)	414 (79%)	74 (14%)	35 (7%)	1	6
All	All	1046/1050 (100%)	822 (79%)	158 (15%)	66 (6%)	1	7

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	407 (91%)	42 (9%)	8	29
1	B	449/449 (100%)	409 (91%)	40 (9%)	9	31
All	All	898/898 (100%)	816 (91%)	82 (9%)	9	30

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TYR
1	A	97	VAL
1	A	109	LEU
1	A	163	TYR
1	A	168	LEU
1	A	187	ARG
1	A	190	THR
1	A	210	LEU
1	A	231	LEU
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	345	ILE
1	A	357	VAL
1	A	381	THR
1	A	388	THR
1	A	390	SER
1	A	397	TRP
1	A	404	THR
1	A	418	VAL
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	526	THR
1	A	539	THR
1	A	550	ILE
1	A	562	ILE
1	A	563	THR
1	A	564	THR
1	B	88	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	117	ASN
1	B	144	MET
1	B	149	LEU
1	B	154	ARG
1	B	163	TYR
1	B	164	GLU
1	B	168	LEU
1	B	172	VAL
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	302	MET
1	B	309	LEU
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	476	LEU
1	B	478	PHE
1	B	526	THR
1	B	550	ILE
1	B	562	ILE
1	B	570	ILE
1	B	584	LEU
1	B	585	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	176	GLN
1	A	193	ASN
1	A	205	GLN
1	A	209	GLN
1	A	257	ASN
1	A	393	GLN
1	A	398	GLN
1	A	474	ASN
1	A	480	ASN
1	A	483	ASN
1	A	531	HIS
1	A	543	ASN
1	B	98	HIS
1	B	147	ASN
1	B	148	GLN
1	B	176	GLN
1	B	193	ASN
1	B	209	GLN
1	B	224	ASN
1	B	228	GLN
1	B	389	GLN
1	B	393	GLN
1	B	398	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	525/525 (100%)	-0.42	0 100 100	16, 31, 60, 85	0
1	B	525/525 (100%)	-0.44	0 100 100	14, 31, 62, 103	0
All	All	1050/1050 (100%)	-0.43	0 100 100	14, 31, 62, 103	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.