



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:03 PM UTC

PDB ID : 4FLN / pdb_00004fln
Title : Crystal structure of plant protease Deg2
Authors : Gong, W.; Liu, L.; Sun, R.; Gao, F.
Deposited on : 2012-06-15
Resolution : 2.80 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

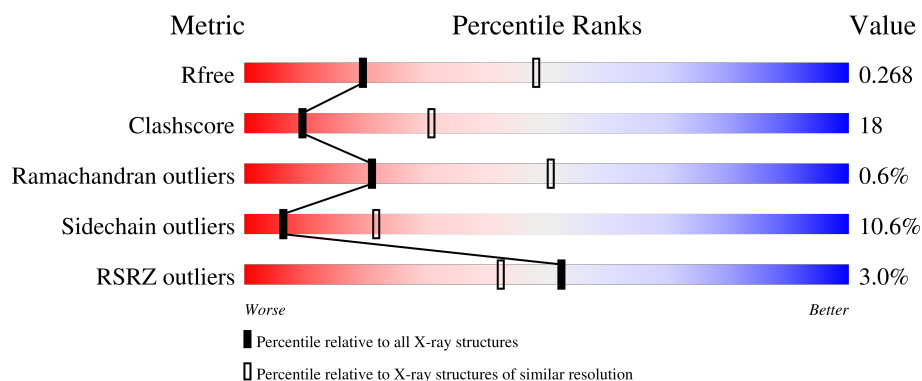
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	539	2% 53% 26% 7% 14%
1	B	539	2% 56% 26% • 14%
1	C	539	3% 53% 29% • 14%
2	D	4	100%
2	F	4	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	20	 90% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10921 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 Protease Do-like 2, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	8	4	0
			3553	2262	613	666	12			
1	B	464	Total	C	N	O	S	0	0	0
			3517	2240	604	661	12			
1	C	463	Total	C	N	O	S	0	2	0
			3506	2236	603	655	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	ASN	-	expression tag	UNP O82261
A	70	ALA	-	expression tag	UNP O82261
B	69	ASN	-	expression tag	UNP O82261
B	70	ALA	-	expression tag	UNP O82261
C	69	ASN	-	expression tag	UNP O82261
C	70	ALA	-	expression tag	UNP O82261

- Molecule 2 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			29	20	5	4			
2	F	4	Total	C	N	O	0	0	0
			29	20	5	4			

- Molecule 3 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	0	0	0
			109	66	21	22			

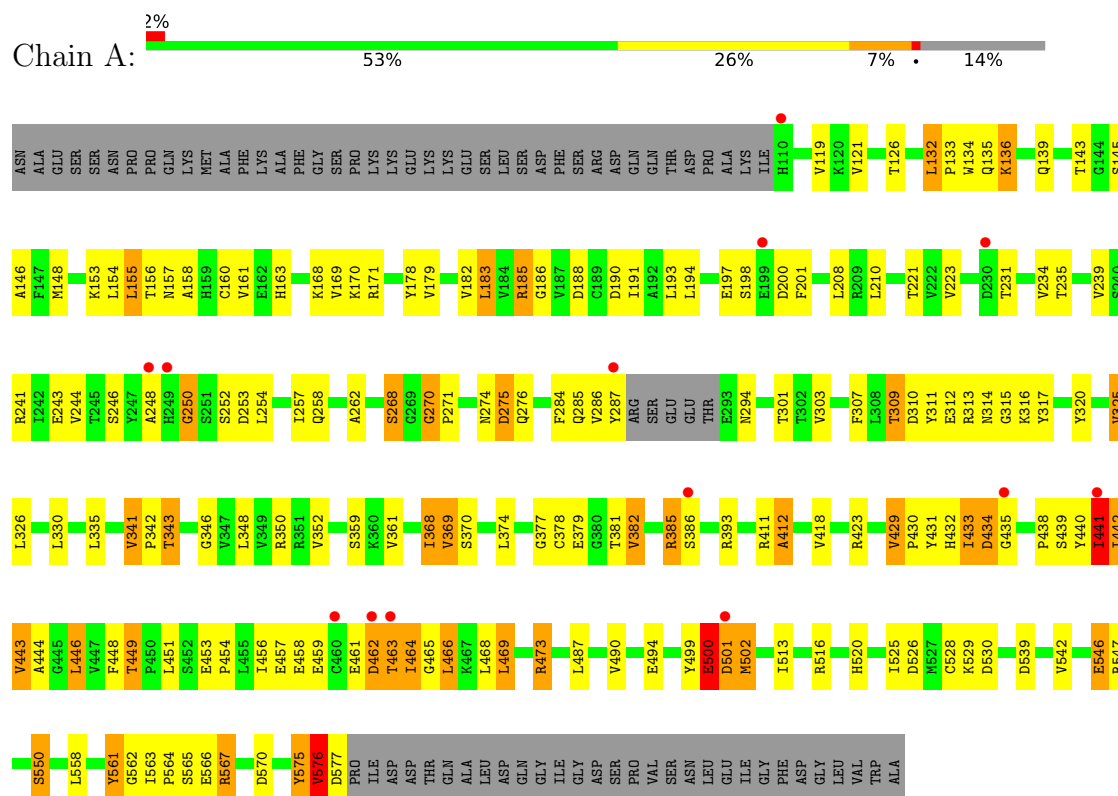
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total 75	O 75	0	0
4	B	61	Total 61	O 61	0	0
4	C	42	Total 42	O 42	0	0

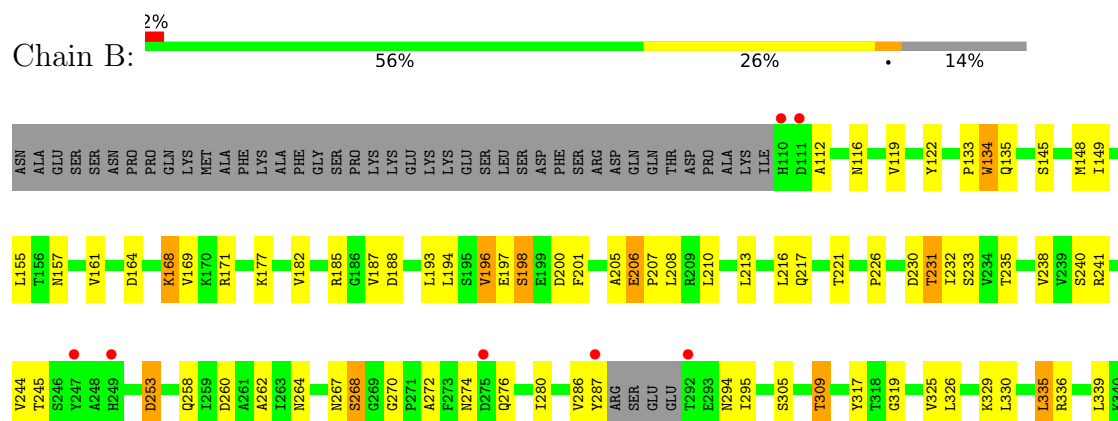
3 Residue-property plots

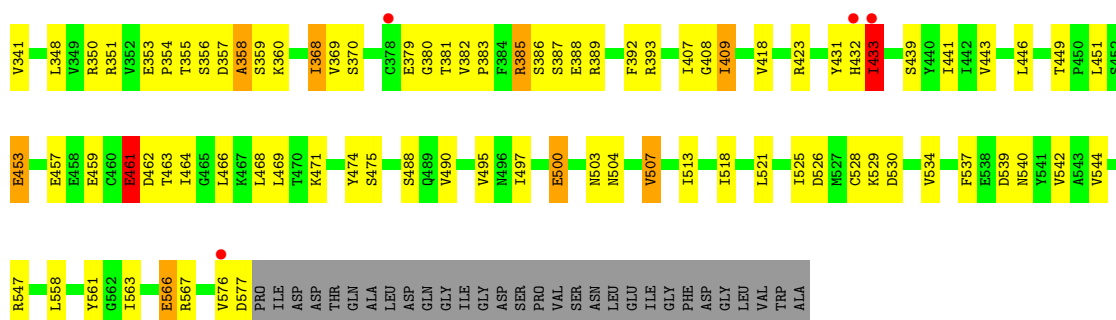
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protease Do-like 2, chloroplastic

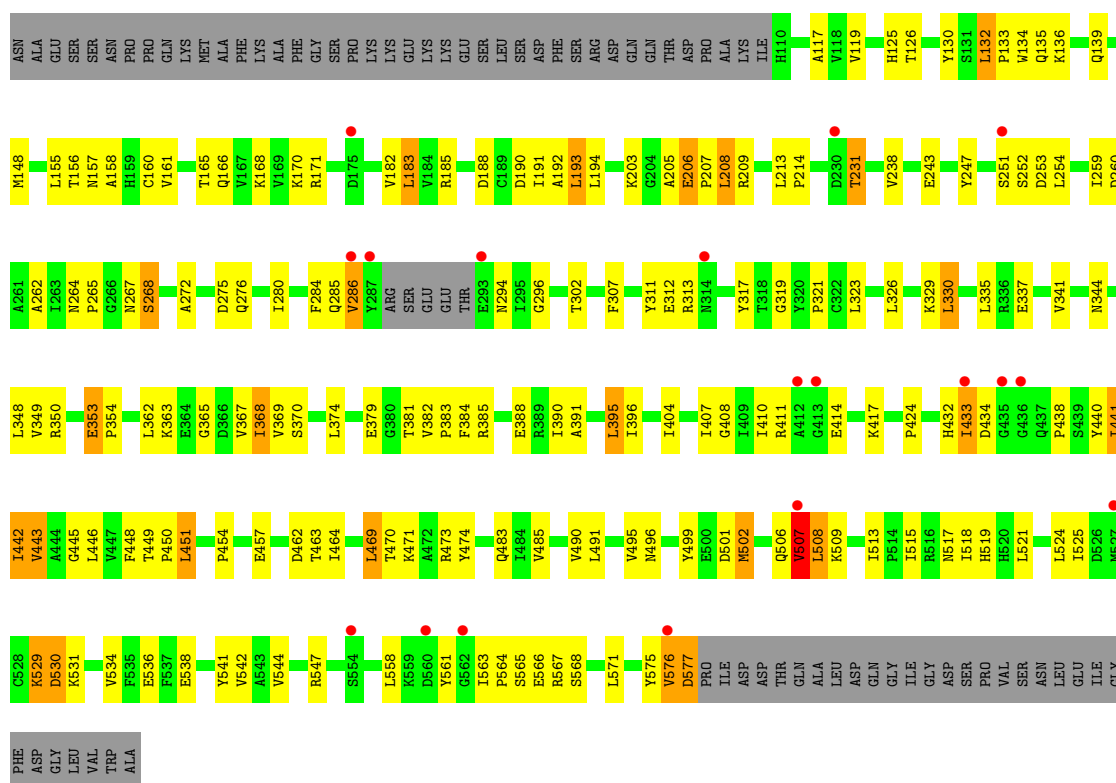


• Molecule 1: Protease Do-like 2, chloroplastic





- Molecule 1: Protease Do-like 2, chloroplastic



- Molecule 2: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 2: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 3: Unknown peptide

Chain E:  90% 10%

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	125.40Å 188.16Å 166.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.80 29.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.74-2.80) 95.6 (29.74-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.274 0.197 , 0.268	Depositor DCC
R_{free} test set	2452 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10921	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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	0.51	0/3634	1.04	27/4941 (0.5%)
1	B	0.45	0/3585	0.94	11/4878 (0.2%)
1	C	0.40	0/3581	0.93	11/4874 (0.2%)
2	D	0.30	0/15	0.42	0/20
2	F	0.23	0/15	0.31	0/20
3	E	0.26	0/22	0.24	0/28
All	All	0.46	0/10852	0.97	49/14761 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
All	All	0	5

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	ILE	N-CA-C	10.84	120.88	111.56
1	A	561	TYR	N-CA-C	10.44	123.93	111.82
1	B	561	TYR	N-CA-C	9.15	122.95	111.69
1	A	132	LEU	CA-C-N	-8.93	112.63	121.65
1	A	132	LEU	C-N-CA	-8.93	112.63	121.65
1	C	561	TYR	N-CA-C	8.90	121.06	111.36
1	A	268	SER	N-CA-C	-7.50	98.71	109.96
1	A	200	ASP	N-CA-C	-7.25	98.47	109.79
1	B	358	ALA	N-CA-C	-6.86	101.68	110.19
1	C	286	VAL	N-CA-C	6.81	117.59	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	507	VAL	N-CA-C	6.68	118.57	112.29
1	C	530	ASP	N-CA-C	6.46	118.20	110.19
1	A	458	GLU	N-CA-C	-6.43	97.10	110.80
1	B	513	ILE	N-CA-C	6.33	114.86	107.77
1	C	353	GLU	CA-C-N	6.17	125.85	119.56
1	C	353	GLU	C-N-CA	6.17	125.85	119.56
1	C	132	LEU	CA-C-N	-6.07	115.52	121.65
1	C	132	LEU	C-N-CA	-6.07	115.52	121.65
1	B	206	GLU	CA-C-N	5.97	126.80	120.11
1	B	206	GLU	C-N-CA	5.97	126.80	120.11
1	A	341	VAL	CA-C-N	5.96	125.67	119.05
1	A	341	VAL	C-N-CA	5.96	125.67	119.05
1	B	213	LEU	CA-C-N	5.96	125.93	120.21
1	B	213	LEU	C-N-CA	5.96	125.93	120.21
1	A	429	VAL	CA-C-N	5.94	125.70	119.76
1	A	429	VAL	C-N-CA	5.94	125.70	119.76
1	A	456	ILE	CA-C-N	-5.88	114.43	123.14
1	A	456	ILE	C-N-CA	-5.88	114.43	123.14
1	A	501	ASP	CB-CA-C	-5.82	109.31	117.23
1	A	381	THR	N-CA-C	5.71	118.71	109.86
1	A	161	VAL	N-CA-C	5.54	117.50	112.29
1	B	461	GLU	N-CA-C	5.50	118.11	111.40
1	A	270	GLY	CA-C-N	5.50	125.97	120.14
1	A	270	GLY	C-N-CA	5.50	125.97	120.14
1	B	500	GLU	N-CA-C	-5.34	103.56	110.19
1	A	513	ILE	N-CA-C	5.31	113.12	107.76
1	A	462	ASP	N-CA-C	-5.30	99.51	110.80
1	A	412	ALA	CB-CA-C	-5.30	110.48	116.63
1	A	382	VAL	CA-C-N	-5.29	114.47	119.76
1	A	382	VAL	C-N-CA	-5.29	114.47	119.76
1	C	206	GLU	CA-C-N	5.25	125.17	119.76
1	C	206	GLU	C-N-CA	5.25	125.17	119.76
1	A	343	THR	CA-C-N	-5.23	116.04	122.84
1	A	343	THR	C-N-CA	-5.23	116.04	122.84
1	B	134	TRP	N-CA-C	-5.17	106.65	113.17
1	A	500	GLU	N-CA-C	-5.14	103.81	110.19
1	A	576	VAL	N-CA-C	5.14	120.04	109.34
1	B	268	SER	N-CA-C	-5.12	102.11	110.20
1	C	268	SER	N-CA-C	-5.11	102.13	110.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	GLY	Peptide
1	A	575	TYR	Peptide
1	C	251	SER	Peptide
1	C	501	ASP	Peptide
1	C	507	VAL	Peptide

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	3553	0	3516	145	1
1	B	3517	0	3457	101	0
1	C	3506	0	3427	138	0
2	D	29	0	15	0	0
2	F	29	0	16	0	0
3	E	109	0	34	2	0
4	A	75	0	0	3	0
4	B	61	0	0	3	0
4	C	42	0	0	4	0
All	All	10921	0	10465	378	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:VAL:HG12	1:C:410:ILE:HD12	1.51	0.91
1:A:526:ASP:OD1	1:A:567:ARG:NH2	2.04	0.89
1:A:461:GLU:HA	1:A:464:ILE:HD11	1.56	0.86
1:A:443:VAL:HG21	1:A:525:ILE:HD13	1.58	0.86
1:C:238:VAL:H	1:C:260:ASP:HB2	1.45	0.82
1:B:576:VAL:HG13	1:B:577:ASP:H	1.46	0.81
1:C:433:ILE:HG12	1:C:454:PRO:HG2	1.62	0.80
1:A:432:HIS:O	1:A:433:ILE:HG13	1.84	0.78
1:C:384:PHE:HD2	1:C:388:GLU:HG2	1.47	0.77
1:B:197:GLU:HA	1:B:198:SER:OG	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:SER:O	1:A:449:THR:HG22	1.85	0.76
1:C:133:PRO:HG2	1:C:440:TYR:HB3	1.68	0.75
1:A:516:ARG:HG3	1:A:520:HIS:ND1	2.02	0.75
1:A:526:ASP:CG	1:A:567:ARG:HH22	1.93	0.75
1:C:135:GLN:NE2	4:C:736:HOH:O	2.20	0.75
1:C:247:TYR:HB2	1:C:252:SER:HB3	1.68	0.75
1:A:119:VAL:HG11	1:A:169:VAL:HB	1.68	0.73
1:C:384:PHE:CD2	1:C:388:GLU:HG2	2.24	0.73
1:B:439:SER:O	1:B:449:THR:HG22	1.89	0.72
1:C:294:ASN:ND2	4:C:709:HOH:O	2.22	0.72
1:B:185:ARG:HD3	4:B:723:HOH:O	1.89	0.72
1:C:350:ARG:HE	1:C:350:ARG:HA	1.55	0.72
1:B:330:LEU:HD21	1:B:348:LEU:HB2	1.70	0.71
1:A:188:ASP:OD1	1:A:317:TYR:OH	2.05	0.71
1:C:509:LYS:HB2	1:C:536:GLU:HB2	1.72	0.71
1:C:529:LYS:O	1:C:547:ARG:NH1	2.24	0.70
1:A:433:ILE:HD12	1:A:435:GLY:H	1.56	0.70
1:C:157:ASN:OD1	1:C:268:SER:HB2	1.91	0.70
1:C:262:ALA:HB2	1:C:294:ASN:HA	1.74	0.69
1:C:350:ARG:HA	1:C:350:ARG:NE	2.07	0.69
1:A:132:LEU:HD22	1:A:134:TRP:CH2	2.28	0.69
1:B:530:ASP:O	1:B:547:ARG:HD3	1.93	0.68
1:B:566:GLU:OE1	1:B:567:ARG:NE	2.28	0.67
1:C:275:ASP:OD1	1:C:276:GLN:NE2	2.26	0.67
1:C:390:ILE:HG13	1:C:391:ALA:H	1.60	0.67
1:C:576:VAL:HG13	1:C:577:ASP:H	1.59	0.67
1:B:241:ARG:HB3	1:B:258:GLN:HB2	1.75	0.67
1:A:148:MET:HE1	1:A:171:ARG:NH1	2.09	0.67
1:C:381:THR:O	1:C:382:VAL:HG23	1.95	0.66
1:C:276:GLN:OE1	4:C:724:HOH:O	2.13	0.66
1:A:155:LEU:HD12	1:A:156:THR:N	2.11	0.66
1:A:221:THR:HG21	1:B:217:GLN:NE2	2.11	0.66
1:A:243:GLU:OE1	1:C:231:THR:HB	1.96	0.66
1:C:132:LEU:HB3	1:C:134:TRP:CZ2	2.30	0.66
1:C:382:VAL:HG11	1:C:395:LEU:HD11	1.76	0.66
1:A:453:GLU:OE2	1:A:473[B]:ARG:NH2	2.28	0.66
1:C:119:VAL:HG23	1:C:171:ARG:HA	1.75	0.66
1:A:462:ASP:C	1:A:464:ILE:H	2.04	0.65
1:A:154:LEU:HB2	1:A:194:LEU:HB2	1.79	0.65
1:C:348:LEU:HD12	1:C:349:VAL:H	1.61	0.65
1:B:526:ASP:CG	1:B:567:ARG:HH22	2.05	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TYR:CD1	1:A:453:GLU:HG2	2.32	0.65
1:A:446:LEU:HB3	1:A:487:LEU:HD11	1.79	0.65
1:B:407:ILE:HG22	1:B:409:ILE:HD13	1.79	0.65
1:A:132:LEU:HD22	1:A:134:TRP:CZ2	2.32	0.65
1:A:575:TYR:CD1	1:A:576:VAL:HG12	2.32	0.64
1:C:161:VAL:HG11	1:C:194:LEU:HD21	1.79	0.64
1:A:253:ASP:OD2	1:A:393:ARG:NH1	2.32	0.63
1:C:442:ILE:O	1:C:446:LEU:O	2.17	0.63
1:B:197:GLU:HA	1:B:198:SER:CB	2.27	0.63
1:C:330:LEU:HB3	1:C:335:LEU:HD12	1.81	0.63
1:A:446:LEU:HB3	1:A:487:LEU:CD1	2.29	0.62
1:C:155:LEU:HD11	1:C:191:ILE:HG23	1.80	0.62
1:A:133:PRO:HG2	1:A:440:TYR:HD2	1.65	0.62
1:A:155:LEU:HD12	1:A:156:THR:H	1.62	0.62
1:B:253:ASP:H	3:E:119:UNK:C	2.13	0.62
1:B:133:PRO:HG3	1:B:449:THR:HG21	1.82	0.62
1:A:441:ILE:O	1:A:566:GLU:O	2.18	0.62
1:B:286:VAL:HG13	1:B:287:TYR:H	1.65	0.62
1:A:155:LEU:HD11	1:A:191:ILE:HG23	1.81	0.61
1:A:241:ARG:HB3	1:A:258:GLN:HB2	1.82	0.61
1:C:441:ILE:HB	1:C:448:PHE:HB2	1.81	0.61
1:A:500:GLU:O	1:A:501:ASP:HB2	2.00	0.61
1:B:446:LEU:HD22	1:B:490:VAL:HG22	1.82	0.61
1:B:149:ILE:HG21	1:B:155:LEU:HD22	1.82	0.61
1:B:380:GLY:O	1:B:392:PHE:HB2	2.01	0.61
1:C:341:VAL:HG11	1:C:367:VAL:HG21	1.82	0.61
1:C:385:ARG:CB	1:C:388:GLU:HB2	2.31	0.61
1:B:245:THR:HG22	4:B:729:HOH:O	2.00	0.60
1:C:507:VAL:HG12	1:C:507:VAL:O	1.99	0.60
1:B:112:ALA:O	1:B:116:ASN:ND2	2.32	0.60
1:A:193:LEU:HD13	1:A:307:PHE:HE2	1.66	0.60
1:A:499:TYR:O	1:A:502:MET:HB2	2.01	0.60
1:C:513:ILE:HG21	1:C:524:LEU:HD11	1.84	0.60
1:A:145:SER:HB2	1:A:270:GLY:N	2.16	0.59
1:A:439:SER:O	1:A:449:THR:CG2	2.49	0.59
1:B:521:LEU:O	1:B:525:ILE:HD13	2.01	0.59
1:B:329:LYS:HD3	1:B:379:GLU:OE1	2.03	0.59
1:A:330:LEU:HD21	1:A:348:LEU:HB2	1.84	0.59
1:C:132:LEU:HD22	1:C:134:TRP:CH2	2.37	0.59
1:B:317:TYR:CZ	1:B:319:GLY:HA2	2.38	0.59
1:C:519:HIS:HD2	1:C:575:TYR:HB2	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:ILE:HG22	1:C:565:SER:H	1.68	0.59
1:B:461:GLU:OE1	1:B:461:GLU:HA	2.02	0.58
1:A:576:VAL:HG22	1:A:577:ASP:H	1.66	0.58
1:A:432:HIS:CE1	1:A:434:ASP:HA	2.38	0.58
1:B:432:HIS:O	1:B:432:HIS:ND1	2.37	0.58
1:A:461:GLU:HA	1:A:464:ILE:CD1	2.30	0.58
1:C:190:ASP:OD1	1:C:284:PHE:HE1	1.87	0.58
1:A:576:VAL:HG22	1:A:577:ASP:N	2.19	0.57
1:C:213:LEU:HD12	1:C:214:PRO:HD2	1.86	0.57
1:A:146:ALA:HB2	1:A:156:THR:HB	1.86	0.57
1:C:563:ILE:HG23	1:C:564:PRO:HD2	1.85	0.57
1:A:442:ILE:O	1:A:446:LEU:O	2.22	0.57
1:A:133:PRO:HG2	1:A:440:TYR:CD2	2.38	0.57
1:A:516:ARG:HG3	1:A:520:HIS:CE1	2.40	0.56
1:B:134:TRP:CG	1:B:563:ILE:HG23	2.41	0.56
1:B:432:HIS:O	1:B:433:ILE:HD12	2.05	0.56
1:A:350:ARG:HA	1:A:350:ARG:NE	2.20	0.56
1:A:352:VAL:HG11	1:A:359:SER:HA	1.87	0.56
1:B:161:VAL:HG11	1:B:194:LEU:HD21	1.86	0.56
1:B:368:ILE:HA	1:B:409:ILE:HD12	1.88	0.56
1:B:462:ASP:C	1:B:464:ILE:H	2.12	0.56
1:C:442:ILE:O	1:C:443:VAL:HB	2.06	0.56
1:C:348:LEU:HD12	1:C:349:VAL:N	2.21	0.56
1:C:502:MET:HE3	1:C:541:TYR:CE2	2.41	0.56
1:B:274:ASN:HB3	1:B:276:GLN:H	1.70	0.56
1:B:576:VAL:HG13	1:B:577:ASP:N	2.19	0.56
1:A:530:ASP:O	1:A:547:ARG:HD3	2.07	0.55
1:B:336:ARG:HG2	1:B:341:VAL:HB	1.87	0.55
1:C:161:VAL:HG23	1:C:185:ARG:NH1	2.21	0.55
1:C:117:ALA:CB	1:C:208:LEU:HD13	2.35	0.55
1:A:133:PRO:CB	1:A:438:PRO:HG2	2.37	0.55
1:C:362:LEU:O	1:C:363:LYS:HG3	2.07	0.55
1:A:262:ALA:HB2	1:A:294:ASN:HA	1.89	0.55
1:A:188:ASP:HB2	1:A:252:SER:OG	2.07	0.54
1:A:274:ASN:HB3	1:A:276:GLN:H	1.72	0.54
1:B:462:ASP:O	1:B:463:THR:OG1	2.18	0.54
1:A:444:ALA:HB2	1:A:550:SER:HB3	1.88	0.54
1:B:335:LEU:HD22	1:B:339:LEU:HD12	1.90	0.54
1:B:336:ARG:CG	1:B:341:VAL:HB	2.37	0.54
1:A:379:GLU:HB2	4:A:769:HOH:O	2.08	0.54
1:A:314:ASN:HB2	4:A:709:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASN:OD1	1:B:268:SER:HB2	2.08	0.54
1:A:183:LEU:CD2	1:A:311:TYR:OH	2.56	0.54
1:A:145:SER:HB2	1:A:270:GLY:H	1.74	0.53
1:C:125:HIS:HE1	1:C:160:CYS:O	1.90	0.53
1:C:508:LEU:HD23	1:C:508:LEU:H	1.73	0.53
1:A:126:THR:HG22	1:A:136:LYS:HD3	1.89	0.53
1:C:490:VAL:HG21	1:C:499:TYR:O	2.08	0.53
1:A:443:VAL:HG21	1:A:525:ILE:CD1	2.36	0.53
1:C:534:VAL:HG22	1:C:544:VAL:HG22	1.91	0.53
1:C:341:VAL:HG23	1:C:341:VAL:O	2.09	0.53
1:A:132:LEU:HB3	1:A:134:TRP:CZ2	2.44	0.52
1:C:567:ARG:CG	1:C:571:LEU:HB2	2.39	0.52
1:A:341:VAL:HG12	1:A:343:THR:O	2.10	0.52
1:A:432:HIS:O	1:A:433:ILE:CG1	2.54	0.52
1:C:183:LEU:HD22	1:C:311:TYR:OH	2.10	0.52
1:B:198:SER:O	1:B:200:ASP:N	2.43	0.52
1:A:464:ILE:HD12	1:A:469:LEU:HD23	1.91	0.52
1:B:385:ARG:HD3	1:B:388:GLU:CD	2.34	0.52
1:C:485:VAL:O	1:C:507:VAL:HG23	2.09	0.52
1:A:576:VAL:HG13	1:A:577:ASP:H	1.73	0.52
1:B:286:VAL:HG13	1:B:287:TYR:N	2.24	0.52
1:C:317:TYR:CZ	1:C:319:GLY:HA2	2.44	0.52
1:A:377:GLY:O	1:A:379:GLU:O	2.26	0.52
1:C:134:TRP:CD1	1:C:135:GLN:HG3	2.44	0.52
1:A:132:LEU:HB3	1:A:134:TRP:CE2	2.45	0.51
1:B:145:SER:HB2	1:B:270:GLY:H	1.75	0.51
1:B:393:ARG:HG2	3:E:118:UNK:H	1.75	0.51
1:C:440:TYR:CD2	1:C:568:SER:HB3	2.45	0.51
1:C:515:ILE:HD13	1:C:521:LEU:HD13	1.93	0.51
1:B:558:LEU:O	1:B:563:ILE:N	2.41	0.51
1:A:562:GLY:C	1:A:563:ILE:HG13	2.35	0.51
1:A:134:TRP:CD1	1:A:135:GLN:HG3	2.47	0.50
1:A:311:TYR:O	1:A:313:ARG:O	2.29	0.50
1:A:461:GLU:CA	1:A:464:ILE:HD11	2.36	0.50
1:A:462:ASP:C	1:A:464:ILE:N	2.70	0.50
1:B:305:SER:O	1:B:309:THR:HG23	2.11	0.50
1:A:313:ARG:O	1:A:315:GLY:N	2.44	0.50
1:C:193:LEU:HD13	1:C:307:PHE:HE2	1.77	0.50
1:A:469:LEU:HD11	1:A:473[A]:ARG:NH2	2.27	0.50
1:A:168:LYS:HA	1:A:178:TYR:O	2.11	0.50
1:C:155:LEU:HD12	1:C:156:THR:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:HH21	1:C:231:THR:H	1.58	0.50
1:C:284:PHE:CZ	1:C:286:VAL:HG13	2.46	0.50
1:C:508:LEU:HD21	1:C:538:GLU:HA	1.94	0.50
1:B:148:MET:SD	1:B:205:ALA:HB1	2.52	0.49
1:A:440:TYR:HA	1:A:448:PHE:O	2.10	0.49
1:C:450:PRO:HD3	1:C:518:ILE:HD12	1.94	0.49
1:B:262:ALA:HB2	1:B:294:ASN:HA	1.95	0.49
1:C:329:LYS:HD2	1:C:379:GLU:HA	1.95	0.49
1:B:534:VAL:HG22	1:B:544:VAL:HG22	1.95	0.49
1:C:441:ILE:HG23	1:C:443:VAL:HG23	1.93	0.49
1:C:383:PRO:O	1:C:384:PHE:HB3	2.13	0.49
1:C:432:HIS:C	1:C:433:ILE:HG13	2.37	0.49
1:B:431:TYR:CE1	1:B:453:GLU:HG2	2.48	0.49
1:C:247:TYR:CE2	1:C:254:LEU:HB2	2.48	0.49
1:A:157:ASN:HB2	1:A:160:CYS:SG	2.53	0.49
1:A:223:VAL:HG22	1:A:234:VAL:HG22	1.94	0.49
1:C:566:GLU:HG3	1:C:567:ARG:N	2.27	0.49
1:A:443:VAL:CG2	1:A:525:ILE:HD13	2.37	0.49
1:B:182:VAL:HG11	1:B:185:ARG:NH2	2.28	0.49
1:B:226:PRO:HG3	1:B:233:SER:OG	2.12	0.49
1:C:368:ILE:O	1:C:368:ILE:HG13	2.11	0.49
1:C:382:VAL:HG11	1:C:395:LEU:CD1	2.43	0.49
1:C:404:ILE:HD12	1:C:404:ILE:N	2.27	0.49
1:B:432:HIS:C	1:B:433:ILE:HD12	2.38	0.49
1:A:268:SER:HB2	1:A:284:PHE:HA	1.94	0.48
1:A:314:ASN:O	1:A:316:LYS:HG2	2.13	0.48
1:C:259:ILE:HG12	1:C:296:GLY:HA3	1.94	0.48
1:C:471:LYS:HD3	1:C:506:GLN:HE22	1.79	0.48
1:C:563:ILE:HG22	1:C:565:SER:N	2.28	0.48
1:C:483:GLN:OE1	1:C:517:ASN:HB2	2.14	0.48
1:A:239:VAL:HG13	1:A:257:ILE:HG23	1.95	0.48
1:C:130:TYR:HE1	1:C:433:ILE:HG23	1.78	0.48
1:C:446:LEU:HD23	1:C:490:VAL:HG13	1.95	0.48
1:C:171:ARG:NH2	1:C:203:LYS:O	2.47	0.48
1:C:321:PRO:HA	1:C:424:PRO:HA	1.96	0.48
1:A:234:VAL:O	1:B:240:SER:HB3	2.13	0.48
1:A:368:ILE:HG13	1:A:369:VAL:N	2.28	0.48
1:B:238:VAL:H	1:B:260:ASP:HB3	1.79	0.48
1:B:149:ILE:HD11	1:B:193:LEU:HD11	1.96	0.48
1:B:507:VAL:HG13	1:B:537:PHE:CE1	2.48	0.48
1:C:253:ASP:O	1:C:254:LEU:HD23	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:LEU:HD13	1:C:565:SER:HA	1.96	0.47
1:C:433:ILE:HG12	1:C:454:PRO:CG	2.40	0.47
1:B:539:ASP:O	1:B:540:ASN:CB	2.62	0.47
1:A:346:GLY:HA2	1:A:368:ILE:O	2.15	0.47
1:B:245:THR:O	1:B:253:ASP:HA	2.14	0.47
1:A:286:VAL:O	1:A:287:TYR:CB	2.62	0.47
1:B:182:VAL:HG11	1:B:185:ARG:CZ	2.44	0.47
1:C:440:TYR:CE2	1:C:568:SER:HB3	2.50	0.47
1:B:463:THR:O	1:B:504:ASN:ND2	2.33	0.47
1:C:344:ASN:O	1:C:344:ASN:ND2	2.48	0.47
1:C:148:MET:SD	1:C:205:ALA:HB1	2.54	0.46
1:A:235:THR:HG22	1:B:260:ASP:OD2	2.14	0.46
1:A:243:GLU:HG3	1:A:244:VAL:N	2.30	0.46
1:B:216:LEU:O	1:B:217:GLN:HB3	2.15	0.46
1:B:264:ASN:O	1:B:267:ASN:HB2	2.16	0.46
1:B:526:ASP:OD1	1:B:567:ARG:NH2	2.46	0.46
1:B:358:ALA:C	1:B:360:LYS:H	2.23	0.46
1:A:119:VAL:CG1	1:A:169:VAL:HB	2.43	0.46
1:A:370:SER:HA	1:A:374:LEU:O	2.16	0.46
1:B:330:LEU:HD22	1:B:335:LEU:HD13	1.97	0.46
1:B:407:ILE:HG22	1:B:409:ILE:CD1	2.45	0.46
1:C:531:LYS:HG3	1:C:531:LYS:O	2.16	0.46
1:A:442:ILE:O	1:A:443:VAL:HB	2.15	0.46
1:C:134:TRP:CZ3	1:C:442:ILE:HD11	2.51	0.46
1:A:182:VAL:HA	1:A:194:LEU:HD23	1.97	0.46
1:B:370:SER:OG	1:B:408:GLY:HA3	2.16	0.46
1:B:471:LYS:O	1:B:475:SER:HB3	2.16	0.46
1:C:265:PRO:HA	1:C:285:GLN:HB3	1.97	0.46
1:A:148:MET:HE1	1:A:171:ARG:HH11	1.79	0.46
1:A:183:LEU:HD21	1:A:311:TYR:OH	2.16	0.45
1:A:361:VAL:CG1	1:A:418:VAL:HB	2.46	0.45
1:B:474:TYR:N	1:B:474:TYR:CD2	2.84	0.45
1:C:442:ILE:O	1:C:443:VAL:CB	2.64	0.45
1:C:390:ILE:HG13	1:C:391:ALA:N	2.29	0.45
1:C:491:LEU:O	1:C:496:ASN:ND2	2.47	0.45
1:A:462:ASP:O	1:A:464:ILE:N	2.49	0.45
1:A:221:THR:HA	1:A:235:THR:O	2.16	0.45
1:B:221:THR:HA	1:B:235:THR:O	2.16	0.45
1:B:350:ARG:HA	1:B:350:ARG:NE	2.31	0.45
1:C:323:LEU:HB2	1:C:396:ILE:HD13	1.98	0.45
1:A:529:LYS:HA	1:A:547:ARG:CZ	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:PRO:CG	1:C:440:TYR:HB3	2.45	0.45
1:A:411:ARG:O	1:A:412:ALA:HB3	2.16	0.45
1:C:170:LYS:NZ	4:C:728:HOH:O	2.49	0.45
1:A:501:ASP:O	1:A:502:MET:C	2.58	0.45
1:B:197:GLU:CA	1:B:198:SER:CB	2.95	0.45
1:B:231:THR:HB	1:C:243:GLU:OE1	2.17	0.45
1:A:330:LEU:O	1:A:378:CYS:HB2	2.16	0.45
1:B:161:VAL:O	1:B:164:ASP:HB3	2.17	0.45
1:B:198:SER:C	1:B:200:ASP:H	2.25	0.45
1:C:567:ARG:HG2	1:C:571:LEU:HB2	1.97	0.45
1:A:275:ASP:OD1	1:A:275:ASP:N	2.39	0.44
1:B:474:TYR:N	1:B:474:TYR:HD2	2.14	0.44
1:C:368:ILE:HD13	1:C:407:ILE:HG23	1.99	0.44
1:A:431:TYR:CE1	1:A:453:GLU:HG2	2.52	0.44
1:B:122:TYR:HB2	1:B:168:LYS:HD2	1.99	0.44
1:C:126:THR:HG22	1:C:136:LYS:HD3	2.00	0.44
1:C:369:VAL:N	1:C:408:GLY:O	2.32	0.44
1:C:348:LEU:HD11	1:C:365:GLY:HA2	2.00	0.44
1:A:576:VAL:HG13	1:A:577:ASP:N	2.32	0.44
1:A:132:LEU:HD13	1:A:134:TRP:CZ2	2.53	0.44
1:C:238:VAL:H	1:C:260:ASP:CB	2.23	0.44
1:C:272:ALA:O	1:C:280:ILE:HG13	2.17	0.44
1:A:563:ILE:HA	1:A:564:PRO:HD3	1.88	0.44
1:C:384:PHE:HB2	1:C:390:ILE:CG2	2.48	0.44
1:C:515:ILE:CD1	1:C:521:LEU:HD13	2.48	0.44
1:A:133:PRO:HB2	1:A:438:PRO:HG2	2.00	0.44
1:B:355:THR:HG23	4:B:726:HOH:O	2.18	0.44
1:C:125:HIS:CE1	1:C:160:CYS:O	2.71	0.44
1:A:561:TYR:N	1:A:562:GLY:HA2	2.33	0.44
1:C:188:ASP:OD1	1:C:188:ASP:N	2.39	0.44
1:A:133:PRO:HB3	1:A:438:PRO:HG2	1.99	0.43
1:A:432:HIS:C	1:A:433:ILE:HG13	2.42	0.43
1:A:464:ILE:HG13	1:A:465:GLY:H	1.83	0.43
1:C:264:ASN:O	1:C:267:ASN:HB2	2.18	0.43
1:A:310:ASP:OD1	1:A:310:ASP:C	2.59	0.43
1:A:185:ARG:NH1	4:A:757:HOH:O	2.30	0.43
1:A:468:LEU:HA	1:A:468:LEU:HD23	1.57	0.43
1:B:357:ASP:C	1:B:358:ALA:O	2.57	0.43
1:A:546:GLU:O	1:A:550:SER:OG	2.35	0.43
1:B:210:LEU:N	1:B:210:LEU:HD23	2.34	0.43
1:C:317:TYR:CE2	1:C:319:GLY:HA2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:HA	1:A:342:PRO:HD3	1.82	0.43
1:C:206:GLU:HA	1:C:207:PRO:HD2	1.86	0.43
1:C:464:ILE:HD13	1:C:464:ILE:HA	1.91	0.43
1:A:186:GLY:HA2	1:A:317:TYR:CD2	2.53	0.43
1:A:268:SER:CB	1:A:285:GLN:H	2.32	0.43
1:B:196:VAL:HG11	1:B:201:PHE:CD2	2.53	0.43
1:B:206:GLU:HA	1:B:207:PRO:HD2	1.90	0.43
1:B:356:SER:O	1:B:358:ALA:O	2.36	0.43
1:B:358:ALA:O	1:B:359:SER:OG	2.27	0.43
1:C:469:LEU:HD21	1:C:473[A]:ARG:CZ	2.48	0.43
1:C:519:HIS:CD2	1:C:575:TYR:HB2	2.50	0.43
1:B:329:LYS:HG2	1:B:379:GLU:HA	2.00	0.43
1:C:133:PRO:HB3	1:C:438:PRO:HG2	2.00	0.43
1:A:182:VAL:HA	1:A:194:LEU:CD2	2.49	0.43
1:A:385:ARG:O	1:A:386:SER:C	2.61	0.43
1:A:431:TYR:CD2	1:A:431:TYR:N	2.86	0.43
1:B:462:ASP:C	1:B:464:ILE:N	2.76	0.42
1:C:353:GLU:HA	1:C:354:PRO:HD3	1.80	0.42
1:C:451:LEU:HD23	1:C:451:LEU:HA	1.78	0.42
1:C:462:ASP:O	1:C:463:THR:CB	2.66	0.42
1:C:513:ILE:CG2	1:C:524:LEU:HD11	2.47	0.42
1:A:223:VAL:O	1:A:271:PRO:HD2	2.20	0.42
1:A:248:ALA:C	1:A:250:GLY:N	2.76	0.42
1:A:303:VAL:HG13	1:A:320:TYR:OH	2.19	0.42
1:B:383:PRO:HD3	1:B:389:ARG:NH2	2.34	0.42
1:B:488:SER:O	1:B:503:ASN:HA	2.19	0.42
1:C:155:LEU:HD12	1:C:156:THR:N	2.34	0.42
1:C:508:LEU:H	1:C:508:LEU:CD2	2.31	0.42
1:A:313:ARG:C	1:A:315:GLY:H	2.27	0.42
1:A:563:ILE:HG23	1:A:564:PRO:HD2	2.01	0.42
1:A:565:SER:OG	1:A:566:GLU:N	2.52	0.42
1:B:253:ASP:OD2	1:B:393:ARG:NH1	2.52	0.42
1:B:528:CYS:SG	1:B:547:ARG:HD2	2.59	0.42
1:A:158:ALA:HB3	1:A:190:ASP:OD1	2.18	0.42
1:A:253:ASP:O	1:A:254:LEU:HD23	2.20	0.42
1:B:188:ASP:OD1	1:B:188:ASP:N	2.43	0.42
1:C:132:LEU:HB3	1:C:134:TRP:CH2	2.54	0.42
1:A:183:LEU:HD22	1:A:311:TYR:OH	2.20	0.42
1:A:210:LEU:HD13	1:A:301:THR:HG23	2.02	0.42
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.74	0.42
1:C:382:VAL:HG13	1:C:383:PRO:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:VAL:C	1:C:507:VAL:HG23	2.45	0.42
1:C:350:ARG:NE	1:C:350:ARG:CA	2.81	0.42
1:C:445:GLY:O	1:C:490:VAL:HA	2.20	0.42
1:B:464:ILE:HD13	1:B:464:ILE:HA	1.89	0.41
1:C:470:THR:O	1:C:474:TYR:HB2	2.20	0.41
1:A:453:GLU:N	1:A:454:PRO:CD	2.82	0.41
1:C:182:VAL:HG11	1:C:185:ARG:CZ	2.51	0.41
1:A:163:HIS:NE2	1:A:433:ILE:HD11	2.35	0.41
1:B:335:LEU:HD23	1:B:335:LEU:HA	1.82	0.41
1:C:441:ILE:CG2	1:C:443:VAL:HG23	2.50	0.41
1:A:309:THR:O	1:A:313:ARG:HG3	2.20	0.41
1:B:134:TRP:CD1	1:B:135:GLN:HG3	2.55	0.41
1:B:353:GLU:HA	1:B:354:PRO:HD3	1.90	0.41
1:A:121:VAL:O	1:A:143:THR:HA	2.20	0.41
1:A:575:TYR:CD2	1:A:575:TYR:O	2.74	0.41
1:C:350:ARG:HE	1:C:350:ARG:CA	2.29	0.41
1:A:325:VAL:HG23	1:A:352:VAL:HG22	2.02	0.41
1:C:168:LYS:HE3	1:C:168:LYS:HB2	1.88	0.41
1:C:473[A]:ARG:HG3	1:C:473[A]:ARG:HH11	1.86	0.41
1:A:153:LYS:HD2	1:A:193:LEU:HD23	2.02	0.41
1:A:462:ASP:C	1:A:463:THR:OG1	2.64	0.41
1:A:528:CYS:O	1:A:529:LYS:HB2	2.21	0.41
1:B:119:VAL:HG11	1:B:169:VAL:HB	2.02	0.41
1:A:440:TYR:CD1	1:A:440:TYR:C	2.99	0.41
1:C:563:ILE:CG2	1:C:565:SER:O	2.69	0.41
1:C:133:PRO:HD3	1:C:449:THR:HG21	2.03	0.40
1:C:158:ALA:HA	1:C:192:ALA:HB2	2.03	0.40
1:A:429:VAL:HA	1:A:430:PRO:HD2	1.89	0.40
1:A:542:VAL:HG13	1:A:542:VAL:O	2.21	0.40
1:A:558:LEU:HB2	1:A:563:ILE:HB	2.03	0.40
1:B:272:ALA:O	1:B:280:ILE:HG13	2.22	0.40
1:B:280:ILE:C	1:B:280:ILE:HD12	2.46	0.40
1:B:441:ILE:HG22	1:B:518:ILE:HD11	2.03	0.40
1:B:497:ILE:HA	1:B:500:GLU:OE2	2.21	0.40
1:C:188:ASP:OD1	1:C:317:TYR:HE2	2.05	0.40
1:C:190:ASP:OD1	1:C:284:PHE:CE1	2.71	0.40
1:A:119:VAL:HG13	1:A:170:LYS:O	2.21	0.40
1:A:154:LEU:HD11	1:A:201:PHE:CZ	2.57	0.40
1:B:286:VAL:O	1:B:287:TYR:CB	2.70	0.40
1:C:381:THR:C	1:C:382:VAL:HG23	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:NE2	1:A:490:VAL:O[3_555]	2.15	0.05

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	463/539 (86%)	423 (91%)	36 (8%)	4 (1%)	14	41
1	B	460/539 (85%)	430 (94%)	29 (6%)	1 (0%)	43	72
1	C	461/539 (86%)	427 (93%)	31 (7%)	3 (1%)	18	47
2	D	1/4 (25%)	1 (100%)	0	0	100	100
2	F	1/4 (25%)	1 (100%)	0	0	100	100
3	E	2/20 (10%)	2 (100%)	0	0	100	100
All	All	1388/1645 (84%)	1284 (92%)	96 (7%)	8 (1%)	21	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	ILE
1	B	433	ILE
1	C	433	ILE
1	A	442	ILE
1	A	576	VAL
1	C	442	ILE
1	A	443	VAL
1	C	443	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	381/463 (82%)	338 (89%)	43 (11%)	5	19
1	B	373/463 (81%)	330 (88%)	43 (12%)	5	18
1	C	367/463 (79%)	332 (90%)	35 (10%)	8	26
2	D	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
3	E	2/2 (100%)	2 (100%)	0	100	100
All	All	1125/1393 (81%)	1004 (89%)	121 (11%)	6	21

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LYS
1	A	155	LEU
1	A	179	VAL
1	A	183	LEU
1	A	185	ARG
1	A	197	GLU
1	A	198	SER
1	A	208	LEU
1	A	231	THR
1	A	246	SER
1	A	275	ASP
1	A	309	THR
1	A	312	GLU
1	A	325	VAL
1	A	326	LEU
1	A	335	LEU
1	A	368	ILE
1	A	369	VAL
1	A	382	VAL
1	A	385	ARG
1	A	423[A]	ARG
1	A	423[B]	ARG
1	A	434	ASP
1	A	441	ILE
1	A	446	LEU
1	A	449	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	451	LEU
1	A	457	GLU
1	A	459	GLU
1	A	463	THR
1	A	464	ILE
1	A	466	LEU
1	A	469	LEU
1	A	473[A]	ARG
1	A	473[B]	ARG
1	A	494	GLU
1	A	500	GLU
1	A	502	MET
1	A	539	ASP
1	A	546	GLU
1	A	550	SER
1	A	567	ARG
1	A	570	ASP
1	B	168	LYS
1	B	171	ARG
1	B	177	LYS
1	B	187	VAL
1	B	196	VAL
1	B	198	SER
1	B	208	LEU
1	B	230	ASP
1	B	231	THR
1	B	232	ILE
1	B	244	VAL
1	B	253	ASP
1	B	295	ILE
1	B	309	THR
1	B	325	VAL
1	B	326	LEU
1	B	335	LEU
1	B	351	ARG
1	B	368	ILE
1	B	369	VAL
1	B	381	THR
1	B	382	VAL
1	B	385	ARG
1	B	386	SER
1	B	387	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	409	ILE
1	B	418	VAL
1	B	423	ARG
1	B	433	ILE
1	B	443	VAL
1	B	451	LEU
1	B	453	GLU
1	B	457	GLU
1	B	459	GLU
1	B	461	GLU
1	B	466	LEU
1	B	468	LEU
1	B	469	LEU
1	B	495	VAL
1	B	507	VAL
1	B	529	LYS
1	B	542	VAL
1	B	566	GLU
1	C	139	GLN
1	C	165	THR
1	C	166	GLN
1	C	183	LEU
1	C	193	LEU
1	C	208	LEU
1	C	209	ARG
1	C	231	THR
1	C	302	THR
1	C	312	GLU
1	C	313	ARG
1	C	326	LEU
1	C	330	LEU
1	C	337	GLU
1	C	368	ILE
1	C	370	SER
1	C	374	LEU
1	C	395	LEU
1	C	411	ARG
1	C	414	GLU
1	C	417	LYS
1	C	434	ASP
1	C	441	ILE
1	C	451	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	457	GLU
1	C	469	LEU
1	C	495	VAL
1	C	502	MET
1	C	508	LEU
1	C	525	ILE
1	C	529	LYS
1	C	530	ASP
1	C	542	VAL
1	C	576	VAL
1	C	577	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	258	GLN
1	A	267	ASN
1	A	398	GLN
1	A	415	HIS
1	A	432	HIS
1	B	139	GLN
1	B	267	ASN
1	B	294	ASN
1	B	314	ASN
1	B	419	GLN
1	B	551	ASN
1	C	166	GLN
1	C	519	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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 ⓘ

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	463/539 (85%)	-0.24	13 (2%)	55 45	26, 53, 93, 140	4 (0%)
1	B	464/539 (86%)	-0.20	11 (2%)	59 49	34, 60, 104, 137	0
1	C	463/539 (85%)	0.11	18 (3%)	43 34	38, 78, 121, 144	2 (0%)
2	D	1/4 (25%)	-0.62	0	100 100	72, 72, 72, 72	0
2	F	1/4 (25%)	-0.64	0	100 100	73, 73, 73, 73	0
3	E	2/20 (10%)	0.13	0	100 100	56, 56, 56, 75	0
All	All	1394/1645 (84%)	-0.11	42 (3%)	52 42	26, 64, 111, 144	6 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	TYR	4.1
1	C	230	ASP	3.9
1	A	248	ALA	3.8
1	A	287	TYR	3.6
1	B	432	HIS	3.5
1	A	460	CYS	3.1
1	A	435	GLY	3.1
1	C	435	GLY	3.1
1	C	412	ALA	3.0
1	B	576	VAL	3.0
1	C	433	ILE	2.9
1	C	293	GLU	2.9
1	C	251	SER	2.9
1	B	433	ILE	2.8
1	C	175	ASP	2.7
1	C	287	TYR	2.7
1	A	199	GLU	2.6
1	C	560	ASP	2.6
1	B	292	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	413	GLY	2.4
1	A	249	HIS	2.4
1	B	378	CYS	2.4
1	C	286	VAL	2.4
1	A	230	ASP	2.4
1	C	576	VAL	2.4
1	A	463	THR	2.4
1	C	314	ASN	2.3
1	B	110	HIS	2.3
1	A	441	ILE	2.3
1	B	249	HIS	2.3
1	B	111	ASP	2.2
1	A	462	ASP	2.2
1	A	110	HIS	2.1
1	C	562	GLY	2.1
1	B	247	TYR	2.1
1	C	554	SER	2.1
1	C	436	GLY	2.1
1	A	501	ASP	2.0
1	B	275	ASP	2.0
1	C	527	MET	2.0
1	A	386	SER	2.0
1	C	507	VAL	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 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.