



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 5XKN / pdb_00005xkn
Title : Crystal structure of plant receptor ERL2 in complexe with EPFL4
Authors : Chai, J.; Lin, G.
Deposited on : 2017-05-08
Resolution : 3.65 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

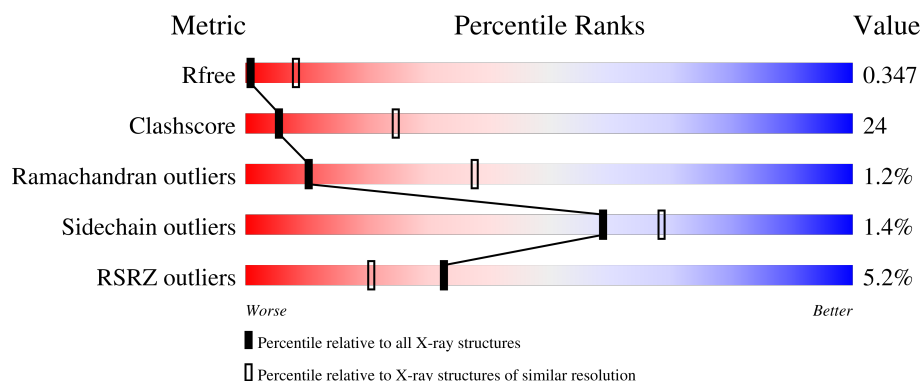
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	E	51	12% 45% 18% • 33%
1	F	51	6% 37% 25% • 33%
2	A	552	3% 64% 32% ...
2	B	552	6% 66% 30% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8824 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 EPIDERMAL PATTERNING FACTOR-like protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	34	Total	C	N	O	S	0	0	0
			269	175	45	45	4			
1	F	34	Total	C	N	O	S	0	0	0
			269	175	45	45	4			

- Molecule 2 is a protein called LRR receptor-like serine/threonine-protein kinase ERL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	540	Total	C	N	O	S	0	0	0
			4143	2646	696	785	16			
2	B	540	Total	C	N	O	S	0	0	0
			4143	2646	696	785	16			

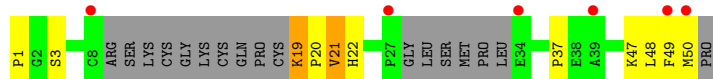
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	HIS	-	expression tag	UNP Q6XAT2
A	577	HIS	-	expression tag	UNP Q6XAT2
A	578	HIS	-	expression tag	UNP Q6XAT2
A	579	HIS	-	expression tag	UNP Q6XAT2
A	580	HIS	-	expression tag	UNP Q6XAT2
A	581	HIS	-	expression tag	UNP Q6XAT2
B	576	HIS	-	expression tag	UNP Q6XAT2
B	577	HIS	-	expression tag	UNP Q6XAT2
B	578	HIS	-	expression tag	UNP Q6XAT2
B	579	HIS	-	expression tag	UNP Q6XAT2
B	580	HIS	-	expression tag	UNP Q6XAT2
B	581	HIS	-	expression tag	UNP Q6XAT2

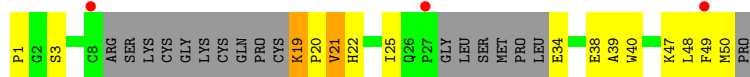
3 Residue-property plots [i](#)

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

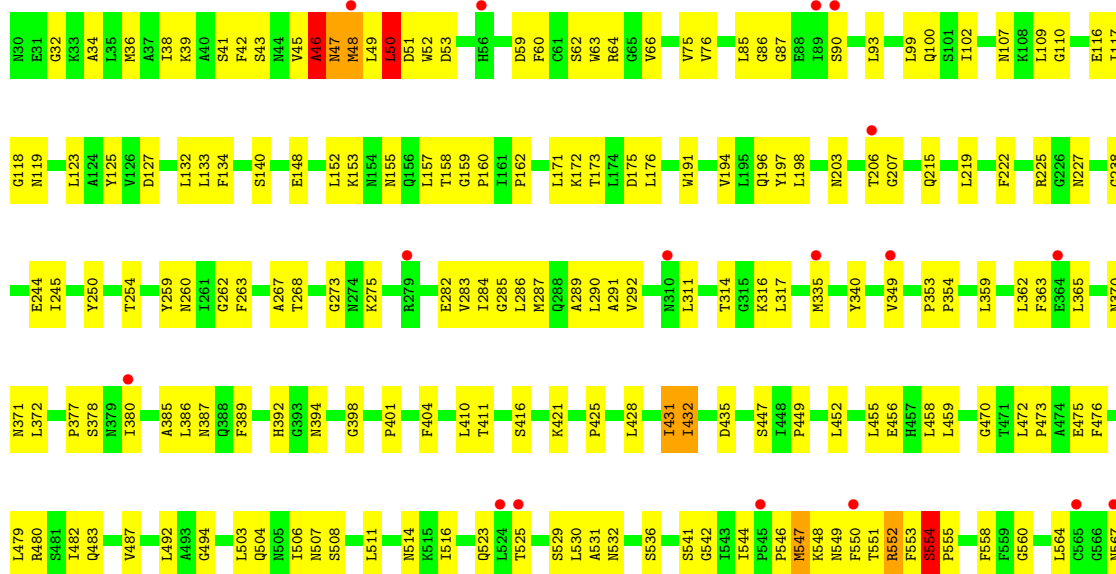
- Molecule 1: EPIDERMAL PATTERNING FACTOR-like protein 4

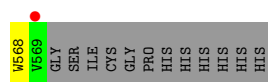


- Molecule 1: EPIDERMAL PATTERNING FACTOR-like protein 4

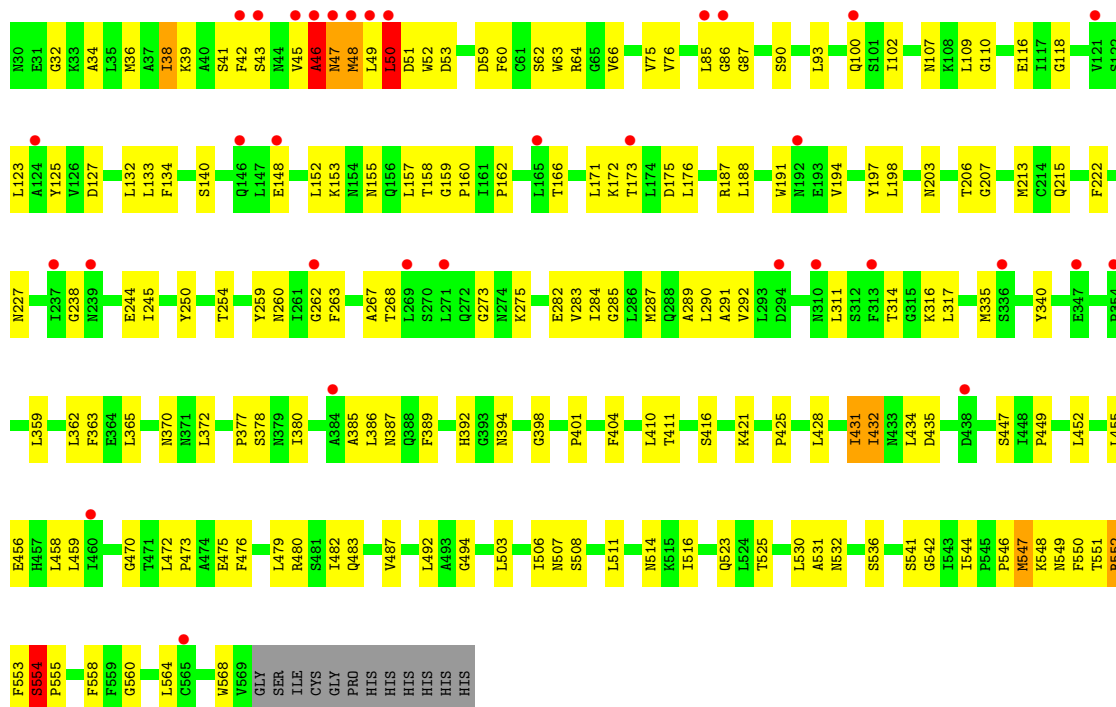


- Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL2





• Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.00Å 112.33Å 175.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 3.65 47.30 – 3.65	Depositor EDS
% Data completeness (in resolution range)	88.7 (47.30-3.65) 88.4 (47.30-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.282 , 0.312 0.337 , 0.347	Depositor DCC
R_{free} test set	1098 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	93.4	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8824	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 [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	E	0.35	0/279	0.76	2/377 (0.5%)
1	F	0.34	0/279	0.76	2/377 (0.5%)
2	A	0.34	0/4224	0.62	6/5750 (0.1%)
2	B	0.34	0/4224	0.63	7/5750 (0.1%)
All	All	0.34	0/9006	0.63	17/12254 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	51	ASP	N-CA-C	10.78	126.11	111.24
2	B	51	ASP	N-CA-C	10.77	126.10	111.24
2	A	554	SER	CA-C-N	9.11	131.23	119.84
2	A	554	SER	C-N-CA	9.11	131.23	119.84
2	B	554	SER	CA-C-N	9.07	131.18	119.84
2	B	554	SER	C-N-CA	9.07	131.18	119.84
2	B	38	ILE	N-CA-C	-8.23	102.02	111.00
2	B	432	ILE	N-CA-C	7.03	123.97	109.34
2	A	432	ILE	N-CA-C	7.03	123.96	109.34
2	B	46	ALA	CB-CA-C	6.36	123.08	110.42
2	A	46	ALA	CB-CA-C	6.35	123.06	110.42
1	E	19	LYS	CA-C-N	5.55	125.75	120.31
1	E	19	LYS	C-N-CA	5.55	125.75	120.31
1	F	19	LYS	CA-C-N	5.52	125.72	120.31
1	F	19	LYS	C-N-CA	5.52	125.72	120.31
2	B	48	MET	N-CA-C	5.34	119.86	113.23
2	A	48	MET	N-CA-C	5.33	119.84	113.23

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	E	269	0	261	16	0
1	F	269	0	261	21	0
2	A	4143	0	4155	203	4
2	B	4143	0	4158	197	4
All	All	8824	0	8835	421	4

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 24.

All (421) 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)
2:B:525:THR:CB	2:B:550:PHE:HZ	1.33	1.40
2:A:525:THR:CB	2:A:550:PHE:CZ	2.04	1.40
2:A:525:THR:CB	2:A:550:PHE:HZ	1.33	1.38
2:B:525:THR:CB	2:B:550:PHE:CZ	2.04	1.36
2:A:554:SER:HB2	2:A:555:PRO:CD	1.59	1.32
2:B:554:SER:HB2	2:B:555:PRO:CD	1.59	1.31
2:A:525:THR:OG1	2:A:550:PHE:CZ	1.77	1.30
2:B:525:THR:OG1	2:B:550:PHE:CZ	1.77	1.28
2:A:525:THR:CG2	2:A:548:LYS:HG3	1.67	1.25
2:B:525:THR:CG2	2:B:548:LYS:HG3	1.67	1.24
2:B:525:THR:HG23	2:B:550:PHE:CZ	1.74	1.23
2:A:525:THR:HG23	2:A:550:PHE:CZ	1.74	1.23
2:B:525:THR:CG2	2:B:550:PHE:CZ	2.22	1.22
2:A:377:PRO:HD2	2:A:380:ILE:CD1	1.68	1.22
2:A:525:THR:CG2	2:A:550:PHE:CZ	2.22	1.22
2:B:377:PRO:HD2	2:B:380:ILE:CD1	1.68	1.22
2:A:553:PHE:O	2:A:558:PHE:CE2	1.94	1.21
2:B:553:PHE:O	2:B:558:PHE:CE2	1.94	1.20
2:A:525:THR:CG2	2:A:550:PHE:HZ	1.56	1.17
2:A:377:PRO:HD2	2:A:380:ILE:HD12	1.19	1.16
2:B:554:SER:CB	2:B:555:PRO:HD2	1.71	1.14
2:B:525:THR:CG2	2:B:550:PHE:HZ	1.57	1.12
2:B:377:PRO:HD2	2:B:380:ILE:HD12	1.19	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:THR:CA	2:B:550:PHE:HZ	1.62	1.11
2:A:525:THR:CA	2:A:550:PHE:HZ	1.62	1.10
2:A:525:THR:CA	2:A:550:PHE:CZ	2.34	1.09
2:A:525:THR:HA	2:A:550:PHE:CZ	1.88	1.09
2:B:525:THR:CA	2:B:550:PHE:CZ	2.34	1.09
2:A:554:SER:CB	2:A:555:PRO:CD	2.25	1.08
2:B:554:SER:CB	2:B:555:PRO:CD	2.25	1.07
2:A:554:SER:CB	2:A:555:PRO:HD2	1.71	1.07
2:B:525:THR:OG1	2:B:550:PHE:CE2	2.08	1.06
2:B:525:THR:HA	2:B:550:PHE:CZ	1.88	1.06
2:A:554:SER:HA	2:A:558:PHE:HE2	1.17	1.06
2:B:525:THR:HA	2:B:550:PHE:CE1	1.91	1.05
2:B:554:SER:HA	2:B:558:PHE:HE2	1.17	1.05
2:A:525:THR:OG1	2:A:550:PHE:CE2	2.08	1.04
2:A:525:THR:HA	2:A:550:PHE:CE1	1.91	1.04
1:E:19:LYS:N	1:E:20:PRO:CD	2.21	1.03
1:F:19:LYS:N	1:F:20:PRO:CD	2.21	1.03
2:B:553:PHE:O	2:B:558:PHE:CZ	2.11	1.03
2:A:525:THR:HG23	2:A:548:LYS:HG3	1.41	1.02
2:A:43:SER:OG	2:A:86:GLY:C	2.03	1.02
2:A:362:LEU:O	2:A:385:ALA:O	1.77	1.02
2:B:362:LEU:O	2:B:385:ALA:O	1.77	1.02
2:B:411:THR:O	2:B:435:ASP:OD1	1.78	1.02
2:A:553:PHE:O	2:A:558:PHE:CZ	2.11	1.01
2:B:525:THR:HG23	2:B:548:LYS:HG3	1.42	1.01
2:A:411:THR:O	2:A:435:ASP:OD1	1.78	1.00
2:B:43:SER:OG	2:B:86:GLY:C	2.03	1.00
2:A:548:LYS:H	2:A:550:PHE:HE2	1.01	0.99
2:A:50:LEU:HD13	2:A:64:ARG:HH11	1.28	0.98
2:A:554:SER:HA	2:A:558:PHE:CE2	1.99	0.97
2:B:554:SER:HA	2:B:558:PHE:CE2	1.99	0.96
2:B:50:LEU:HD13	2:B:64:ARG:HH11	1.28	0.96
2:A:48:MET:O	2:A:50:LEU:HD12	1.67	0.95
2:A:50:LEU:CD1	2:A:64:ARG:NH1	2.30	0.95
2:B:48:MET:O	2:B:50:LEU:HD12	1.67	0.95
2:B:50:LEU:CD1	2:B:64:ARG:NH1	2.30	0.94
2:B:45:VAL:HG22	2:B:85:LEU:HD22	1.49	0.94
2:A:525:THR:HG23	2:A:550:PHE:CE2	2.03	0.94
2:B:525:THR:CG2	2:B:550:PHE:CE2	2.50	0.94
2:B:525:THR:HG23	2:B:550:PHE:CE2	2.03	0.94
2:A:525:THR:CG2	2:A:550:PHE:CE2	2.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:34:ALA:O	2:A:38:ILE:HG12	1.69	0.93
2:A:287:MET:HA	1:F:3:SER:OG	1.68	0.93
2:B:34:ALA:O	2:B:38:ILE:HG12	1.69	0.92
1:E:19:LYS:N	1:E:20:PRO:HD2	1.84	0.92
2:A:50:LEU:CD1	2:A:64:ARG:HH11	1.83	0.92
1:F:19:LYS:N	1:F:20:PRO:HD2	1.84	0.92
2:A:45:VAL:HG22	2:A:85:LEU:HD22	1.49	0.92
2:B:50:LEU:CD1	2:B:64:ARG:HH11	1.83	0.91
2:B:548:LYS:H	2:B:550:PHE:HE2	1.01	0.91
2:A:525:THR:CG2	2:A:548:LYS:CG	2.50	0.89
2:B:525:THR:CG2	2:B:548:LYS:CG	2.50	0.88
2:A:531:ALA:O	2:A:553:PHE:HZ	1.58	0.86
2:B:50:LEU:HD11	2:B:64:ARG:NH1	1.91	0.86
2:B:50:LEU:HD13	2:B:64:ARG:NH1	1.91	0.86
2:B:531:ALA:O	2:B:553:PHE:HZ	1.58	0.85
2:A:50:LEU:HD11	2:A:64:ARG:NH1	1.91	0.85
2:B:43:SER:OG	2:B:87:GLY:N	2.09	0.85
2:A:554:SER:O	2:A:558:PHE:CD2	2.30	0.85
2:A:43:SER:OG	2:A:87:GLY:N	2.09	0.85
2:B:377:PRO:HD2	2:B:380:ILE:HD11	1.57	0.85
2:B:554:SER:O	2:B:558:PHE:CD2	2.30	0.84
2:B:525:THR:HG22	2:B:548:LYS:HG3	1.58	0.84
2:A:377:PRO:HD2	2:A:380:ILE:HD11	1.57	0.84
2:A:525:THR:HG22	2:A:548:LYS:HG3	1.58	0.84
2:A:554:SER:HB2	2:A:555:PRO:HD2	0.87	0.84
2:A:48:MET:O	2:A:50:LEU:CD1	2.25	0.84
2:B:48:MET:O	2:B:50:LEU:CD1	2.25	0.84
2:B:554:SER:HB2	2:B:555:PRO:HD2	0.87	0.83
1:F:48:LEU:HG	1:F:49:PHE:H	1.42	0.83
1:E:48:LEU:HG	1:E:49:PHE:H	1.42	0.83
2:B:377:PRO:CD	2:B:380:ILE:CD1	2.56	0.83
2:A:377:PRO:CD	2:A:380:ILE:CD1	2.56	0.82
2:B:45:VAL:CG1	2:B:49:LEU:HD23	2.10	0.82
2:A:50:LEU:HD13	2:A:64:ARG:NH1	1.91	0.82
2:B:41:SER:OG	2:B:90:SER:HB2	1.81	0.81
2:A:45:VAL:CG1	2:A:49:LEU:HD23	2.10	0.81
2:B:531:ALA:C	2:B:553:PHE:HZ	1.89	0.81
2:A:377:PRO:CD	2:A:380:ILE:HD12	2.06	0.80
2:B:45:VAL:HG12	2:B:49:LEU:HD23	1.61	0.80
2:A:531:ALA:C	2:A:553:PHE:HZ	1.89	0.80
2:A:45:VAL:HG12	2:A:49:LEU:HD23	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:41:SER:OG	2:A:90:SER:HB2	1.81	0.80
2:A:45:VAL:O	2:A:47:ASN:N	2.15	0.80
2:B:548:LYS:N	2:B:550:PHE:CE2	2.50	0.80
2:A:548:LYS:N	2:A:550:PHE:CE2	2.50	0.80
2:B:45:VAL:O	2:B:47:ASN:N	2.15	0.79
2:A:45:VAL:C	2:A:47:ASN:N	2.37	0.79
2:A:554:SER:O	2:A:558:PHE:HD2	1.66	0.78
2:B:45:VAL:C	2:B:47:ASN:N	2.37	0.77
2:B:377:PRO:CD	2:B:380:ILE:HD12	2.06	0.77
2:B:554:SER:O	2:B:558:PHE:HD2	1.66	0.76
1:F:48:LEU:HG	1:F:49:PHE:N	2.01	0.74
2:A:525:THR:HA	2:A:550:PHE:HE1	1.54	0.72
2:A:268:THR:OG1	1:F:38:GLU:O	2.06	0.72
2:A:50:LEU:HD11	2:A:64:ARG:HH12	1.54	0.72
2:B:50:LEU:HD11	2:B:64:ARG:HH12	1.54	0.71
1:E:48:LEU:HG	1:E:49:PHE:N	2.01	0.70
2:B:380:ILE:HG22	2:B:380:ILE:O	1.90	0.69
2:B:45:VAL:C	2:B:47:ASN:H	1.97	0.69
2:A:380:ILE:O	2:A:380:ILE:HG22	1.90	0.69
2:A:45:VAL:C	2:A:47:ASN:H	1.97	0.69
1:F:19:LYS:N	1:F:20:PRO:HD3	2.08	0.68
2:A:45:VAL:CG1	2:A:49:LEU:HB3	2.24	0.67
2:A:525:THR:HG23	2:A:548:LYS:CG	2.21	0.67
2:B:45:VAL:CG1	2:B:49:LEU:HB3	2.24	0.67
2:B:377:PRO:CD	2:B:380:ILE:HD11	2.24	0.67
1:E:19:LYS:N	1:E:20:PRO:HD3	2.08	0.67
2:B:525:THR:HA	2:B:550:PHE:HE1	1.54	0.67
2:A:43:SER:O	2:A:45:VAL:N	2.28	0.66
2:A:377:PRO:CD	2:A:380:ILE:HD11	2.24	0.66
2:B:363:PHE:O	2:B:386:LEU:HD12	1.96	0.66
2:A:206:THR:HG22	2:A:207:GLY:H	1.61	0.66
2:A:456:GLU:OE1	2:A:480:ARG:NH2	2.29	0.65
2:B:43:SER:O	2:B:45:VAL:N	2.28	0.65
1:E:3:SER:OG	2:B:287:MET:HA	1.96	0.65
2:B:45:VAL:CB	2:B:49:LEU:HD23	2.26	0.65
2:B:544:ILE:HD11	2:B:568:TRP:HH2	1.62	0.65
2:B:206:THR:HG22	2:B:207:GLY:H	1.61	0.65
2:A:544:ILE:HD11	2:A:568:TRP:HH2	1.62	0.64
2:B:531:ALA:O	2:B:553:PHE:CZ	2.46	0.64
2:A:244:GLU:O	2:A:267:ALA:N	2.31	0.64
2:A:363:PHE:O	2:A:386:LEU:HD12	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:VAL:CB	2:A:49:LEU:HD23	2.26	0.64
2:A:52:TRP:NE1	2:A:63:TRP:HB3	2.12	0.64
2:B:525:THR:HG23	2:B:548:LYS:CG	2.21	0.64
2:A:508:SER:HA	2:A:532:ASN:O	1.98	0.64
2:A:363:PHE:HE1	2:A:385:ALA:HB1	1.63	0.63
2:B:363:PHE:HE1	2:B:385:ALA:HB1	1.63	0.63
2:A:245:ILE:HD12	1:F:25:ILE:HD11	1.78	0.63
2:B:52:TRP:NE1	2:B:63:TRP:HB3	2.12	0.63
2:B:158:THR:HG22	2:B:159:GLY:H	1.63	0.63
2:B:456:GLU:OE1	2:B:480:ARG:NH2	2.29	0.63
2:B:363:PHE:CE1	2:B:385:ALA:HB1	2.34	0.63
2:A:45:VAL:HG11	2:A:49:LEU:HB3	1.82	0.62
2:A:158:THR:HG22	2:A:159:GLY:H	1.64	0.62
2:A:531:ALA:O	2:A:553:PHE:CZ	2.46	0.62
2:B:244:GLU:O	2:B:267:ALA:N	2.31	0.62
2:B:508:SER:HA	2:B:532:ASN:O	1.98	0.62
2:A:363:PHE:CE1	2:A:385:ALA:HB1	2.34	0.62
2:A:125:TYR:HE2	2:A:127:ASP:HB2	1.65	0.61
2:B:45:VAL:HG11	2:B:49:LEU:HB3	1.82	0.61
2:B:125:TYR:HE2	2:B:127:ASP:HB2	1.65	0.61
2:A:49:LEU:HD12	2:A:49:LEU:O	2.01	0.61
2:B:49:LEU:HD12	2:B:49:LEU:O	2.01	0.61
2:A:173:THR:HG23	2:A:197:TYR:HB3	1.83	0.60
1:E:1:PRO:HA	2:B:263:PHE:CE1	2.36	0.60
2:A:45:VAL:HB	2:A:49:LEU:HD23	1.83	0.60
2:A:118:GLY:HA3	2:A:140:SER:HB3	1.84	0.59
2:B:45:VAL:HB	2:B:49:LEU:HD23	1.83	0.59
2:B:554:SER:CB	2:B:555:PRO:HD3	2.26	0.59
2:B:118:GLY:HA3	2:B:140:SER:HB3	1.84	0.59
1:F:48:LEU:CG	1:F:49:PHE:H	2.15	0.59
2:B:259:TYR:CE1	2:B:283:VAL:HG11	2.37	0.59
2:A:316:LYS:HG2	2:A:340:TYR:HD2	1.68	0.59
2:B:531:ALA:C	2:B:553:PHE:CZ	2.77	0.59
2:A:259:TYR:CE1	2:A:283:VAL:HG11	2.37	0.59
2:B:173:THR:HG23	2:B:197:TYR:HB3	1.83	0.59
2:B:554:SER:HB2	2:B:555:PRO:HD3	1.74	0.59
2:B:42:PHE:CG	2:B:43:SER:N	2.69	0.59
1:E:48:LEU:CG	1:E:49:PHE:H	2.15	0.59
2:A:554:SER:CB	2:A:555:PRO:HD3	2.26	0.58
2:B:431:ILE:HG22	2:B:431:ILE:O	2.03	0.58
2:A:431:ILE:HG22	2:A:431:ILE:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:LYS:HG2	2:B:340:TYR:HD2	1.68	0.57
2:A:531:ALA:C	2:A:553:PHE:CZ	2.77	0.57
2:B:370:ASN:HB2	2:B:394:ASN:HD21	1.70	0.57
2:A:34:ALA:O	2:A:38:ILE:CG1	2.49	0.57
2:B:172:LYS:HG2	2:B:194:VAL:HG12	1.86	0.56
2:B:525:THR:CG2	2:B:550:PHE:HE2	2.17	0.56
2:A:551:THR:HG22	2:A:551:THR:O	2.04	0.56
2:A:290:LEU:O	2:A:314:THR:HG22	2.06	0.56
2:A:370:ASN:HB2	2:A:394:ASN:HD21	1.70	0.56
2:B:42:PHE:CD2	2:B:43:SER:N	2.74	0.56
2:A:42:PHE:CD2	2:A:43:SER:N	2.74	0.55
2:A:245:ILE:CD1	1:F:25:ILE:HD11	2.36	0.55
2:A:172:LYS:HG2	2:A:194:VAL:HG12	1.86	0.55
2:A:483:GLN:HA	2:A:506:ILE:HA	1.88	0.55
2:B:483:GLN:HA	2:B:506:ILE:HA	1.88	0.55
2:A:42:PHE:CG	2:A:43:SER:N	2.69	0.55
2:B:45:VAL:O	2:B:48:MET:N	2.39	0.55
2:B:551:THR:O	2:B:551:THR:HG22	2.04	0.55
2:A:292:VAL:HG13	2:A:316:LYS:HB2	1.88	0.55
2:B:377:PRO:HB2	2:B:380:ILE:HG13	1.89	0.55
2:B:290:LEU:O	2:B:314:THR:HG22	2.06	0.55
2:B:292:VAL:HG13	2:B:316:LYS:HB2	1.88	0.55
2:A:45:VAL:O	2:A:48:MET:N	2.39	0.55
2:B:285:GLY:HA2	2:B:311:LEU:HD11	1.89	0.54
2:A:377:PRO:HB2	2:A:380:ILE:HG13	1.89	0.54
2:B:380:ILE:O	2:B:380:ILE:CG2	2.56	0.54
2:B:32:GLY:O	2:B:36:MET:HG2	2.08	0.54
1:F:21:VAL:HG13	1:F:22:HIS:N	2.23	0.54
2:A:473:PRO:HG2	2:A:476:PHE:HE1	1.72	0.53
2:B:34:ALA:O	2:B:38:ILE:CG1	2.49	0.53
2:B:473:PRO:HG2	2:B:476:PHE:HE1	1.72	0.53
2:A:50:LEU:HD12	2:A:50:LEU:N	2.24	0.53
2:A:263:PHE:CE1	1:F:1:PRO:HA	2.43	0.53
2:B:50:LEU:HD12	2:B:50:LEU:N	2.24	0.53
1:E:21:VAL:HG13	1:E:22:HIS:N	2.23	0.53
2:A:267:ALA:CB	1:F:39:ALA:HA	2.37	0.53
2:A:289:ALA:O	1:F:40:TRP:NE1	2.40	0.53
2:A:285:GLY:HA2	2:A:311:LEU:HD11	1.89	0.53
2:B:268:THR:HG23	2:B:292:VAL:HB	1.90	0.53
2:B:387:ASN:O	2:B:410:LEU:HD12	2.09	0.53
2:A:38:ILE:HD11	2:A:93:LEU:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:268:THR:HG23	2:A:292:VAL:HB	1.90	0.52
2:A:387:ASN:O	2:A:410:LEU:HD12	2.09	0.52
2:B:38:ILE:HD11	2:B:93:LEU:N	2.24	0.52
2:A:32:GLY:O	2:A:36:MET:HG2	2.08	0.52
2:A:287:MET:CA	1:F:3:SER:OG	2.49	0.52
2:A:473:PRO:HG2	2:A:476:PHE:CE1	2.45	0.52
2:B:472:LEU:HD12	2:B:473:PRO:HD2	1.91	0.52
2:B:523:GLN:OE1	2:B:523:GLN:N	2.40	0.52
2:A:250:TYR:CD1	2:A:273:GLY:HA3	2.45	0.52
2:B:50:LEU:HB2	2:B:64:ARG:HB2	1.92	0.52
2:B:39:LYS:HD3	2:B:52:TRP:HB2	1.91	0.51
2:A:52:TRP:CD1	2:A:63:TRP:HB3	2.45	0.51
2:B:473:PRO:HG2	2:B:476:PHE:CE1	2.45	0.51
1:E:48:LEU:CG	1:E:49:PHE:N	2.73	0.51
2:A:380:ILE:O	2:A:380:ILE:CG2	2.56	0.51
2:A:50:LEU:HB2	2:A:64:ARG:HB2	1.92	0.51
2:A:267:ALA:HB3	1:F:39:ALA:HA	1.92	0.51
2:B:250:TYR:CD1	2:B:273:GLY:HA3	2.45	0.51
2:B:363:PHE:HE1	2:B:385:ALA:CB	2.23	0.51
2:B:552:ARG:CG	2:B:552:ARG:NH2	2.74	0.51
2:A:377:PRO:CG	2:A:380:ILE:HD11	2.41	0.51
2:B:554:SER:CA	2:B:558:PHE:CE2	2.85	0.51
2:A:554:SER:HB2	2:A:555:PRO:HD3	1.74	0.51
2:A:455:LEU:HD12	2:A:458:LEU:HD22	1.93	0.51
2:A:472:LEU:HD12	2:A:473:PRO:HD2	1.91	0.51
2:B:455:LEU:HD12	2:B:458:LEU:HD22	1.93	0.51
2:B:52:TRP:CD1	2:B:63:TRP:HB3	2.45	0.51
2:A:363:PHE:HE1	2:A:385:ALA:CB	2.23	0.50
2:A:372:LEU:H	2:A:394:ASN:HD22	1.60	0.50
2:B:45:VAL:HG12	2:B:49:LEU:HB3	1.93	0.50
2:B:377:PRO:CG	2:B:380:ILE:HD11	2.41	0.50
2:A:401:PRO:HG2	2:A:404:PHE:HE1	1.77	0.50
2:A:552:ARG:CG	2:A:552:ARG:NH2	2.74	0.50
2:A:392:HIS:ND1	2:A:416:SER:OG	2.41	0.50
2:A:45:VAL:HG12	2:A:49:LEU:HB3	1.93	0.50
2:B:449:PRO:HB2	2:B:452:LEU:HD13	1.93	0.50
2:A:554:SER:CA	2:A:558:PHE:CE2	2.85	0.49
2:B:479:LEU:O	2:B:482:ILE:HG22	2.12	0.49
2:B:372:LEU:H	2:B:394:ASN:HD22	1.60	0.49
2:A:41:SER:OG	2:A:41:SER:O	2.28	0.49
2:A:50:LEU:CD1	2:A:50:LEU:N	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:449:PRO:HB2	2:A:452:LEU:HD13	1.93	0.49
2:A:425:PRO:O	2:A:428:LEU:HG	2.13	0.49
2:A:59:ASP:OD2	2:A:62:SER:OG	2.21	0.49
2:A:377:PRO:HG2	2:A:380:ILE:HD11	1.95	0.49
2:A:479:LEU:O	2:A:482:ILE:HG22	2.12	0.49
2:B:548:LYS:N	2:B:550:PHE:CD2	2.81	0.49
2:A:191:TRP:CZ3	2:A:215:GLN:HG2	2.48	0.48
2:B:401:PRO:HG2	2:B:404:PHE:HE1	1.77	0.48
2:A:548:LYS:N	2:A:550:PHE:CD2	2.81	0.48
2:B:525:THR:HG21	2:B:548:LYS:CG	2.42	0.48
2:A:262:GLY:HA2	2:A:287:MET:SD	2.54	0.48
2:B:45:VAL:HG12	2:B:49:LEU:CD2	2.38	0.48
2:A:45:VAL:O	2:A:46:ALA:C	2.57	0.48
2:B:262:GLY:HA2	2:B:287:MET:SD	2.54	0.48
2:A:191:TRP:CE3	2:A:215:GLN:HG2	2.48	0.48
2:A:401:PRO:HG2	2:A:404:PHE:CE1	2.49	0.48
2:B:191:TRP:CE3	2:B:215:GLN:HG2	2.48	0.48
2:B:377:PRO:HG2	2:B:380:ILE:HD11	1.95	0.48
2:A:472:LEU:HD13	2:A:492:LEU:HD23	1.96	0.48
2:B:191:TRP:CZ3	2:B:215:GLN:HG2	2.48	0.48
2:B:398:GLY:HA2	2:B:421:LYS:HE2	1.96	0.48
2:B:425:PRO:O	2:B:428:LEU:HG	2.13	0.48
2:B:50:LEU:CD1	2:B:50:LEU:N	2.76	0.48
2:A:398:GLY:HA2	2:A:421:LYS:HE2	1.96	0.47
2:A:523:GLN:OE1	2:A:523:GLN:N	2.40	0.47
2:B:507:ASN:HA	2:B:530:LEU:HA	1.96	0.47
2:B:401:PRO:HG2	2:B:404:PHE:CE1	2.49	0.47
2:A:45:VAL:HG12	2:A:49:LEU:CD2	2.38	0.47
2:B:267:ALA:HA	2:B:289:ALA:O	2.15	0.47
2:B:39:LYS:HD2	2:B:49:LEU:HD13	1.97	0.47
2:A:541:SER:OG	2:A:542:GLY:N	2.48	0.47
2:B:472:LEU:HD13	2:B:492:LEU:HD23	1.96	0.47
2:A:507:ASN:HA	2:A:530:LEU:HA	1.96	0.47
2:A:554:SER:HB3	2:A:555:PRO:CD	2.38	0.47
2:B:213:MET:HE2	2:B:213:MET:HB3	1.76	0.47
2:B:536:SER:HB2	2:B:560:GLY:H	1.79	0.47
2:A:525:THR:CG2	2:A:550:PHE:HE2	2.17	0.46
2:B:45:VAL:O	2:B:46:ALA:C	2.57	0.46
2:B:133:LEU:N	2:B:155:ASN:OD1	2.46	0.46
2:A:317:LEU:HD22	2:A:335:MET:HE1	1.96	0.46
2:A:536:SER:HB2	2:A:560:GLY:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ASP:OD2	2:B:62:SER:OG	2.21	0.46
2:B:392:HIS:ND1	2:B:416:SER:OG	2.41	0.46
2:A:284:ILE:HA	2:A:287:MET:HG3	1.97	0.46
2:A:66:VAL:HG23	2:A:75:VAL:HG13	1.97	0.46
2:B:148:GLU:HA	2:B:171:LEU:HA	1.98	0.46
2:B:267:ALA:O	2:B:291:ALA:N	2.32	0.46
2:B:317:LEU:HD22	2:B:335:MET:HE1	1.96	0.46
1:F:49:PHE:O	1:F:50:MET:HG3	2.16	0.46
2:B:541:SER:OG	2:B:542:GLY:N	2.48	0.45
2:A:267:ALA:HA	2:A:289:ALA:O	2.15	0.45
2:B:284:ILE:HA	2:B:287:MET:HG3	1.97	0.45
1:E:49:PHE:O	1:E:49:PHE:CD1	2.69	0.45
2:A:148:GLU:HA	2:A:171:LEU:HA	1.98	0.45
2:B:203:ASN:O	2:B:227:ASN:HA	2.17	0.45
1:F:49:PHE:O	1:F:49:PHE:CD1	2.69	0.45
2:A:43:SER:O	2:A:45:VAL:HG23	2.17	0.45
1:F:21:VAL:CG1	1:F:22:HIS:N	2.79	0.45
2:A:198:LEU:HD23	2:A:222:PHE:HE1	1.81	0.45
2:B:282:GLU:H	2:B:282:GLU:CD	2.24	0.45
2:B:494:GLY:O	2:B:516:ILE:HG23	2.17	0.45
2:A:39:LYS:HD2	2:A:49:LEU:HD13	1.91	0.45
2:A:203:ASN:O	2:A:227:ASN:HA	2.17	0.45
2:A:282:GLU:H	2:A:282:GLU:CD	2.24	0.45
2:A:494:GLY:O	2:A:516:ILE:HG23	2.17	0.45
2:A:133:LEU:N	2:A:155:ASN:OD1	2.46	0.45
2:B:66:VAL:HG23	2:B:75:VAL:HG13	1.97	0.44
1:E:21:VAL:CG1	1:E:22:HIS:N	2.79	0.44
2:A:45:VAL:HG22	2:A:85:LEU:CD2	2.34	0.44
2:B:43:SER:O	2:B:45:VAL:HG23	2.17	0.44
2:B:359:LEU:HB3	2:B:362:LEU:HB2	1.99	0.44
2:A:63:TRP:HB2	2:A:66:VAL:CG1	2.47	0.44
2:B:198:LEU:HD23	2:B:222:PHE:HE1	1.81	0.44
2:A:482:ILE:HG21	2:A:503:LEU:HD13	1.99	0.44
2:B:134:PHE:HA	2:B:157:LEU:HA	2.00	0.44
1:E:49:PHE:O	1:E:50:MET:HG3	2.16	0.44
2:B:39:LYS:HD2	2:B:49:LEU:CD1	2.47	0.44
2:A:45:VAL:HG12	2:A:49:LEU:CB	2.48	0.44
2:B:63:TRP:HB2	2:B:66:VAL:CG1	2.47	0.43
2:B:198:LEU:HD23	2:B:222:PHE:CE1	2.53	0.43
2:B:116:GLU:CD	2:B:116:GLU:H	2.26	0.43
2:B:152:LEU:HB2	2:B:176:LEU:HD23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:152:LEU:HB2	2:A:176:LEU:HD23	2.00	0.43
2:B:45:VAL:HG12	2:B:49:LEU:CB	2.48	0.43
2:A:198:LEU:HD23	2:A:222:PHE:CE1	2.53	0.43
2:B:482:ILE:HG21	2:B:503:LEU:HD13	1.99	0.43
2:B:547:MET:HB2	2:B:550:PHE:HE2	1.83	0.43
2:B:60:PHE:HA	2:B:63:TRP:CE2	2.53	0.43
2:B:250:TYR:HD1	2:B:273:GLY:HA3	1.84	0.43
2:A:547:MET:HB2	2:A:550:PHE:HE2	1.84	0.43
2:A:134:PHE:HA	2:A:157:LEU:HA	2.00	0.43
2:A:254:THR:HG22	2:A:275:LYS:HB2	2.01	0.43
2:A:365:LEU:HD23	2:A:389:PHE:HE1	1.83	0.43
2:B:45:VAL:HG22	2:B:85:LEU:CD2	2.34	0.43
2:B:45:VAL:HG12	2:B:45:VAL:O	2.19	0.43
2:B:254:THR:HG22	2:B:275:LYS:HB2	2.01	0.43
2:B:160:PRO:O	2:B:162:PRO:HD3	2.19	0.43
2:A:525:THR:HG21	2:A:548:LYS:CG	2.42	0.43
2:A:45:VAL:CG2	2:A:85:LEU:HD22	2.35	0.42
2:B:365:LEU:HD23	2:B:389:PHE:HE1	1.83	0.42
2:A:359:LEU:HB3	2:A:362:LEU:HB2	1.99	0.42
2:B:107:ASN:HB2	2:B:109:LEU:HG	2.02	0.42
2:A:116:GLU:H	2:A:116:GLU:CD	2.26	0.42
2:B:45:VAL:HG12	2:B:49:LEU:H	1.85	0.42
1:E:37:PRO:HB2	2:B:245:ILE:HD13	2.01	0.42
2:A:110:GLY:HA2	2:A:132:LEU:O	2.19	0.42
2:A:153:LYS:HE3	2:A:175:ASP:OD2	2.19	0.42
2:B:153:LYS:HE3	2:B:175:ASP:OD2	2.19	0.42
2:B:487:VAL:HG22	2:B:511:LEU:HD22	2.02	0.42
2:A:504:GLN:O	2:A:529:SER:OG	2.29	0.42
2:A:353:PRO:HA	2:A:354:PRO:HD3	1.87	0.42
2:A:472:LEU:HD13	2:A:492:LEU:CD2	2.49	0.42
2:B:110:GLY:HA2	2:B:132:LEU:O	2.20	0.42
2:A:60:PHE:HA	2:A:63:TRP:CE2	2.53	0.42
2:A:160:PRO:O	2:A:162:PRO:HD3	2.19	0.42
2:B:447:SER:HB3	2:B:470:GLY:HA3	2.02	0.42
2:B:459:LEU:HA	2:B:482:ILE:HA	2.02	0.42
2:A:99:LEU:HD23	2:A:99:LEU:HA	1.91	0.42
2:A:459:LEU:HA	2:A:482:ILE:HA	2.02	0.42
2:A:492:LEU:HB2	2:A:514:ASN:OD1	2.19	0.42
2:B:45:VAL:CG2	2:B:85:LEU:HD22	2.35	0.42
2:B:102:ILE:HD11	2:B:123:LEU:HD11	2.02	0.42
2:B:472:LEU:HD13	2:B:492:LEU:CD2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:250:TYR:HD1	2:A:273:GLY:HA3	1.84	0.41
2:A:475:GLU:CD	2:A:475:GLU:H	2.27	0.41
2:B:492:LEU:HB2	2:B:514:ASN:OD1	2.19	0.41
2:B:564:LEU:HD12	2:B:564:LEU:HA	1.85	0.41
2:A:36:MET:HE1	2:A:53:ASP:N	2.36	0.41
2:A:117:ILE:C	2:A:119:ASN:H	2.29	0.41
2:B:36:MET:HE1	2:B:53:ASP:N	2.36	0.41
2:A:107:ASN:HB2	2:A:109:LEU:HG	2.02	0.41
2:A:45:VAL:HG12	2:A:49:LEU:H	1.84	0.41
2:A:238:GLY:HA3	2:A:260:ASN:HB3	2.02	0.41
2:B:238:GLY:HA3	2:B:260:ASN:HB3	2.02	0.41
2:B:475:GLU:H	2:B:475:GLU:CD	2.27	0.41
2:A:102:ILE:HD11	2:A:123:LEU:HD11	2.02	0.41
2:B:39:LYS:CD	2:B:49:LEU:HD13	2.51	0.41
2:B:554:SER:HB3	2:B:555:PRO:CD	2.38	0.41
1:E:1:PRO:HA	2:B:263:PHE:CD1	2.55	0.41
2:A:45:VAL:HG12	2:A:45:VAL:O	2.19	0.41
2:A:76:VAL:O	2:A:100:GLN:HB2	2.21	0.41
2:A:196:GLN:C	2:A:219:LEU:HD12	2.46	0.41
2:A:225:ARG:NH2	1:F:34:GLU:CG	2.84	0.41
2:A:487:VAL:HG22	2:A:511:LEU:HD22	2.02	0.41
2:A:564:LEU:HD12	2:A:564:LEU:HA	1.85	0.41
1:E:3:SER:OG	2:B:287:MET:CA	2.67	0.40
2:A:267:ALA:O	2:A:291:ALA:N	2.32	0.40
2:B:76:VAL:O	2:B:100:GLN:HB2	2.21	0.40
2:A:447:SER:HB3	2:A:470:GLY:HA3	2.02	0.40
2:B:166:THR:HG21	2:B:188:LEU:HG	2.04	0.40
2:A:286:LEU:O	1:F:3:SER:N	2.47	0.40
2:B:434:LEU:HA	2:B:434:LEU:HD23	1.85	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:349:VAL:CG1	2:B:187:ARG:NE[2_555]	1.63	0.57
2:A:349:VAL:CG1	2:B:187:ARG:CZ[2_555]	1.90	0.30
2:A:567:ASN:O	2:B:48:MET:SD[3_645]	1.95	0.25
2:A:371:ASN:CB	2:B:187:ARG:NH1[2_555]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	28/51 (55%)	23 (82%)	4 (14%)	1 (4%)	2	19
1	F	28/51 (55%)	23 (82%)	4 (14%)	1 (4%)	2	19
2	A	538/552 (98%)	476 (88%)	56 (10%)	6 (1%)	11	39
2	B	538/552 (98%)	476 (88%)	56 (10%)	6 (1%)	11	39
All	All	1132/1206 (94%)	998 (88%)	120 (11%)	14 (1%)	10	38

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	46	ALA
2	A	546	PRO
2	B	46	ALA
2	B	546	PRO
2	A	432	ILE
2	B	432	ILE
2	A	50	LEU
2	B	50	LEU
1	E	47	LYS
1	F	47	LYS
2	A	547	MET
2	B	547	MET
2	A	554	SER
2	B	554	SER

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	E	31/46 (67%)	30 (97%)	1 (3%)	34	54
1	F	31/46 (67%)	30 (97%)	1 (3%)	34	54
2	A	471/481 (98%)	465 (99%)	6 (1%)	61	69
2	B	471/481 (98%)	465 (99%)	6 (1%)	61	69
All	All	1004/1054 (95%)	990 (99%)	14 (1%)	59	68

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	21	VAL
2	A	47	ASN
2	A	50	LEU
2	A	378	SER
2	A	431	ILE
2	A	549	ASN
2	A	552	ARG
2	B	47	ASN
2	B	50	LEU
2	B	378	SER
2	B	431	ILE
2	B	549	ASN
2	B	552	ARG
1	F	21	VAL

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

Mol	Chain	Res	Type
2	A	74	ASN
2	A	82	ASN
2	A	227	ASN
2	A	252	GLN
2	A	310	ASN
2	A	320	HIS
2	A	344	ASN
2	A	387	ASN
2	A	394	ASN
2	A	433	ASN
2	A	505	ASN
2	A	549	ASN
2	B	74	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	82	ASN
2	B	227	ASN
2	B	252	GLN
2	B	310	ASN
2	B	320	HIS
2	B	344	ASN
2	B	387	ASN
2	B	394	ASN
2	B	433	ASN
2	B	505	ASN
2	B	549	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	E	34/51 (66%)	0.79	6 (17%) 4 4	76, 106, 157, 165	0
1	F	34/51 (66%)	0.87	3 (8%) 15 12	76, 106, 157, 165	0
2	A	540/552 (97%)	0.28	18 (3%) 49 29	78, 104, 150, 171	0
2	B	540/552 (97%)	0.60	33 (6%) 27 17	78, 104, 150, 171	0
All	All	1148/1206 (95%)	0.47	60 (5%) 33 21	76, 104, 150, 171	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	47	ASN	6.1
2	B	48	MET	4.9
1	E	49	PHE	4.6
2	B	460	ILE	4.4
2	B	86	GLY	3.8
2	A	569	VAL	3.6
1	F	27	PRO	3.4
2	B	42	PHE	3.3
2	B	262	GLY	3.2
1	F	49	PHE	3.2
2	B	46	ALA	3.2
2	B	100	GLN	3.0
2	B	565	CYS	3.0
2	A	206	THR	3.0
2	B	165	LEU	3.0
2	B	336	SER	2.9
2	A	89	ILE	2.9
1	E	39	ALA	2.9
2	B	45	VAL	2.8
2	B	384	ALA	2.8
2	B	49	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	85	LEU	2.7
2	B	173	THR	2.7
2	A	524	LEU	2.7
2	B	121	VAL	2.6
2	A	545	PRO	2.6
2	B	310	ASN	2.6
2	A	90	SER	2.5
2	B	271	LEU	2.5
2	A	349	VAL	2.5
1	E	27	PRO	2.5
2	B	269	LEU	2.5
2	A	567	ASN	2.5
2	A	550	PHE	2.4
2	A	525	THR	2.4
2	A	565	CYS	2.4
2	B	43	SER	2.4
2	B	124	ALA	2.3
2	B	313	PHE	2.3
2	A	335	MET	2.3
1	E	34	GLU	2.3
2	A	56	HIS	2.3
2	A	380	ILE	2.2
2	B	192	ASN	2.2
2	B	438	ASP	2.2
2	A	48	MET	2.2
2	B	50	LEU	2.2
2	B	239	ASN	2.2
2	B	354	PRO	2.2
2	A	310	ASN	2.1
2	B	294	ASP	2.1
1	E	8	CYS	2.1
2	B	146	GLN	2.1
2	A	279	ARG	2.1
2	B	237	ILE	2.1
1	E	50	MET	2.1
2	B	347	GLU	2.1
1	F	8	CYS	2.1
2	A	364	GLU	2.0
2	B	148	GLU	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.