Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 04:11 PM JST

PDB ID	:	5XKJ
Title	:	Crystal structure of plant receptor ERL1-TMM in complexe with EPF2
Authors	:	Chai, J.; Lin, G.
Deposited on	:	2017-05-07
Resolution	:	3.48 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:

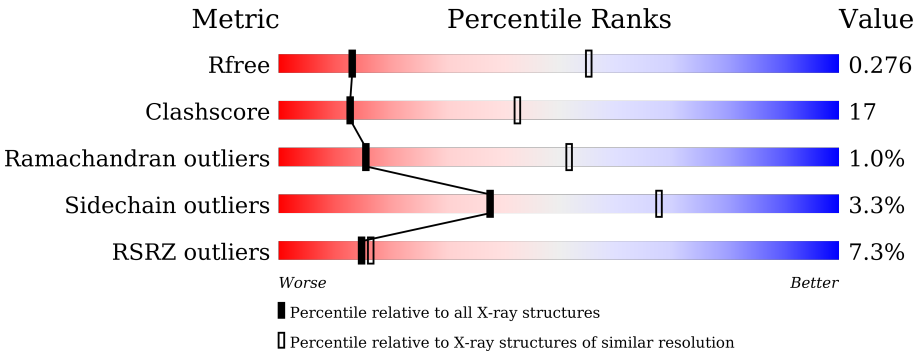
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 <=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	C	433	3% 57% 26% • 16%
1	D	433	4% 58% 25% • 16%
2	E	52	10% 35% 40% 6% 6% 13%
2	F	52	13% 29% 46% 6% 6% 13%
3	A	555	8% 65% 26% • 8%
3	B	555	9% 64% 27% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14174 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein TOO MANY MOUTHS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	363	Total	C	N	O	S	0	0	0
			2827	1784	511	522	10			
1	D	363	Total	C	N	O	S	0	0	0
			2827	1784	511	522	10			

- Molecule 2 is a protein called Protein EPIDERMAL PATTERNING FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	45	Total	C	N	O	S	0	0	0
			340	209	63	60	8			
2	F	45	Total	C	N	O	S	0	0	0
			340	209	63	60	8			

- Molecule 3 is a protein called LRR receptor-like serine/threonine-protein kinase ERL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	513	Total	C	N	O	S	0	0	0
			3920	2487	666	752	15			
3	B	513	Total	C	N	O	S	0	0	0
			3920	2487	666	752	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	HIS	-	expression tag	UNP C0LGW6
A	574	HIS	-	expression tag	UNP C0LGW6
A	575	HIS	-	expression tag	UNP C0LGW6
A	576	HIS	-	expression tag	UNP C0LGW6
A	577	HIS	-	expression tag	UNP C0LGW6
A	578	HIS	-	expression tag	UNP C0LGW6
B	573	HIS	-	expression tag	UNP C0LGW6
B	574	HIS	-	expression tag	UNP C0LGW6

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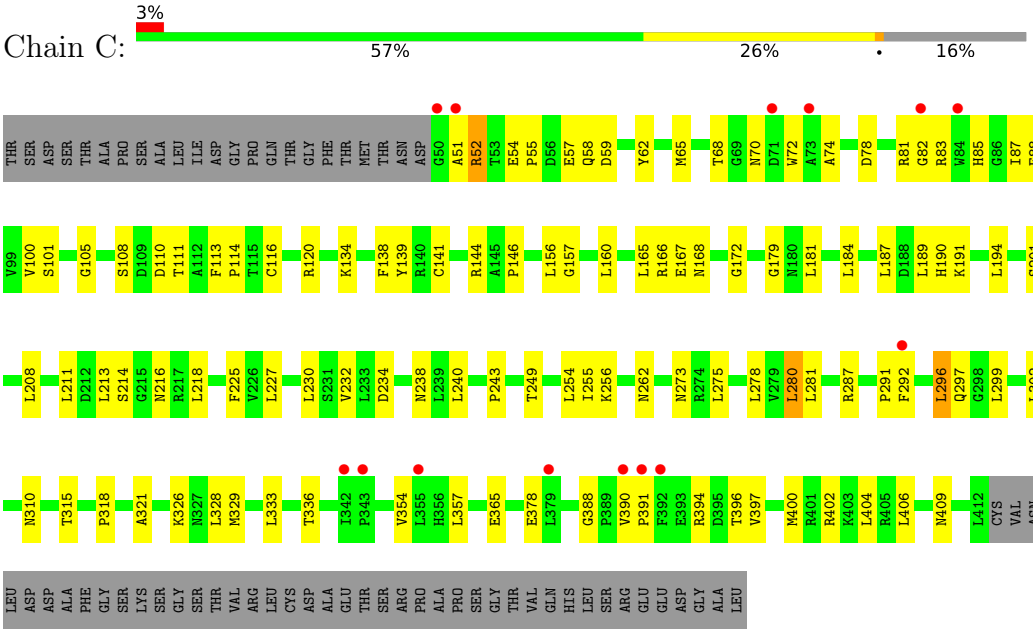
Chain	Residue	Modelled	Actual	Comment	Reference
B	575	HIS	-	expression tag	UNP C0LGW6
B	576	HIS	-	expression tag	UNP C0LGW6
B	577	HIS	-	expression tag	UNP C0LGW6
B	578	HIS	-	expression tag	UNP C0LGW6

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.

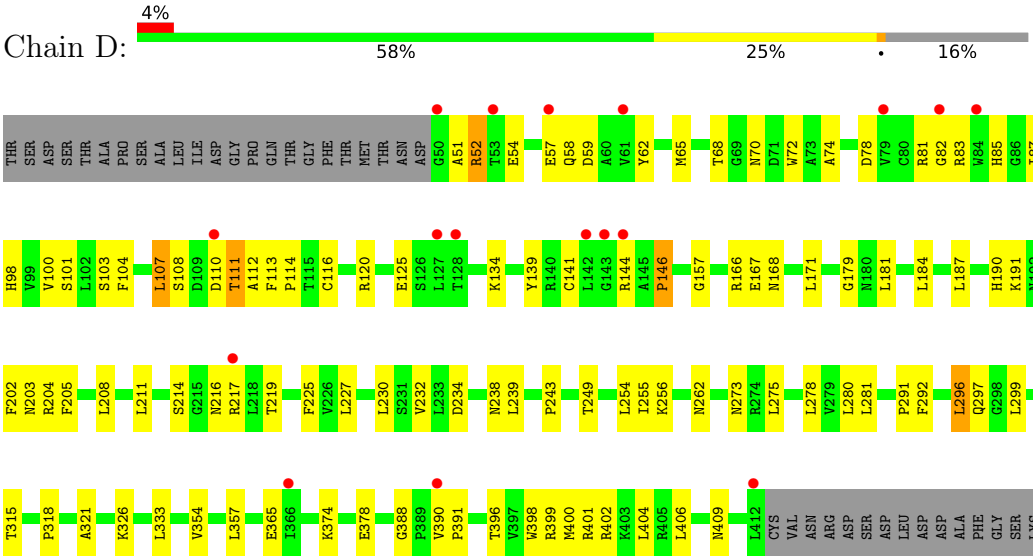
• Molecule 1: Protein TOO MANY MOUTHS

Chain C:

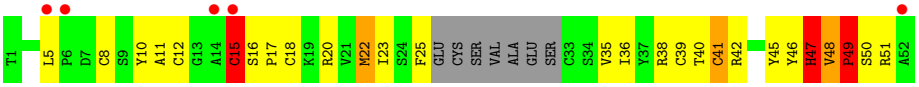


• Molecule 1: Protein TOO MANY MOUTHS

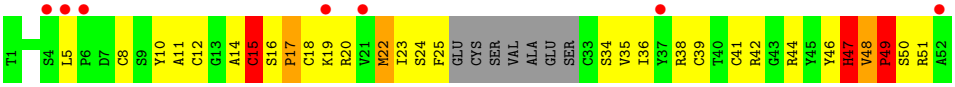
Chain D:



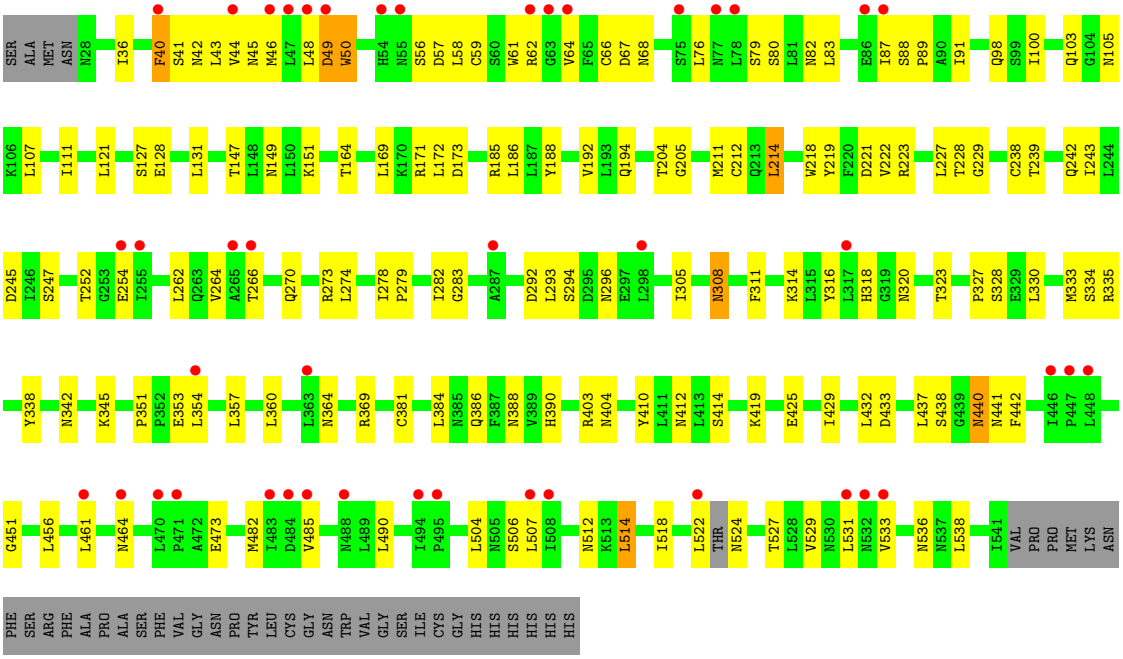
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 2



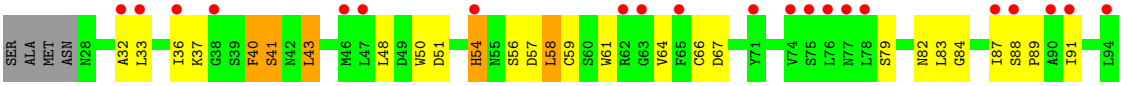
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 2

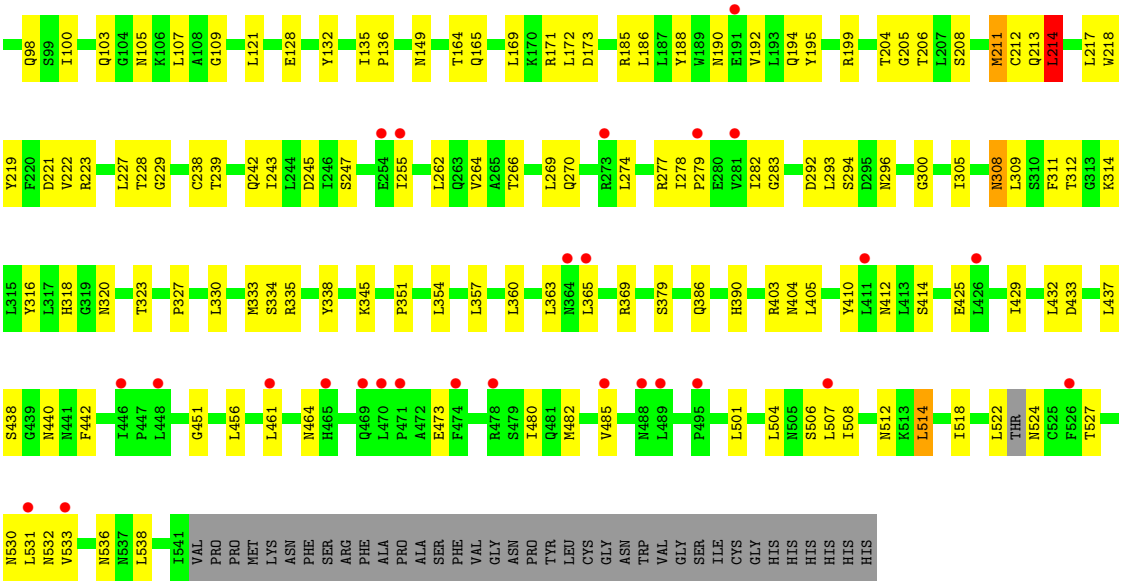


• Molecule 3: LRR receptor-like serine/threonine-protein kinase ERL1



• Molecule 3: LRR receptor-like serine/threonine-protein kinase ERL1




Q98 S99 I100 Q103 G104 N105 K106 L107 A108 G109 L121 E128 Y132 I135 P136 N149 T164 Q165 L169 K170 R171 L172 D173 R185 L186 L187 Y188 W189 N190 E191 V192 L193 Q194 Y195 R199 T204 G205 T206 L207 S208 M211 C212 Q213 L214 L217 W218
Y219 F220 D221 V222 R223 L227 T228 G229 C238 T239 Q242 I243 L244 D245 I246 S247 E254 I255 L262 Q263 V264 A265 T266 L269 Q270 R273 L274 R277 I278 P279 E280 V281 I282 G283 D292 L293 S294 D296 N296 G300 I305 N308 L309 S310 F311 T312 G313 K314
L315 Y316 L317 H318 G319 N320 T323 P327 L330 M333 S334 R335 Y338 K345 P351 L354 L357 L360 L363 N364 L365 R369 S379 Q386 H390 R403 N404 L405 Y410 L411 N412 L413 S414 E425 L426 I429 L432 D433 L437
S438 G439 N440 N441 F442 I446 P447 L448 G451 L456 L461 N464 H465 Q469 L470 P471 A472 E473 F474 R478 S479 I480 Q481 M482 V485 N488 L489 P495 L501 L504 N505 S506 L507 I508 N512 K513 L514 I518 L522 THR N524 G525 F526 T527
N530 L531 N532 V533 N536 N537 L538 I541 VAL PRO PRO MET LYS ASN PHE SER ARG PHE ALA PRO ALA SER PHE VAL GLY ASN PRO TYR LEU CYS GLY ASN TRP VAL GLY SER ILE CYS GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.15Å 65.60Å 142.50Å 102.86° 97.60° 93.58°	Depositor
Resolution (Å)	46.19 – 3.48 47.91 – 3.48	Depositor EDS
% Data completeness (in resolution range)	94.7 (46.19-3.48) 94.8 (47.91-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.254 , 0.277 0.254 , 0.276	Depositor DCC
R_{free} test set	1420 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , -1.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	14174	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	C	0.31	0/2883	0.54	0/3915
1	D	0.32	0/2883	0.54	0/3915
2	E	0.53	0/347	0.90	2/466 (0.4%)
2	F	0.60	0/347	0.91	1/466 (0.2%)
3	A	0.35	0/3985	0.53	0/5419
3	B	0.34	0/3985	0.55	1/5419 (0.0%)
All	All	0.35	0/14430	0.56	4/19600 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	15	CYS	CA-CB-SG	7.09	126.76	114.00
3	B	214	LEU	N-CA-C	-6.97	92.17	111.00
2	E	15	CYS	CA-CB-SG	6.02	124.84	114.00
2	E	49	PRO	CB-CA-C	-5.00	99.49	112.00

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	C	2827	0	2875	79	1
1	D	2827	0	2875	113	1
2	E	340	0	327	36	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	340	0	327	62	0
3	A	3920	0	3971	124	1
3	B	3920	0	3972	127	2
All	All	14174	0	14347	473	3

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 17.

All (473) 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)
3:B:59:CYS:SG	3:B:66:CYS:CB	2.23	1.24
1:D:111:THR:CG2	3:B:194:GLN:OE1	1.89	1.20
1:D:193:HIS:O	1:D:217:ARG:NH1	1.76	1.19
3:A:59:CYS:SG	3:A:66:CYS:SG	1.20	1.16
3:B:41:SER:OG	3:B:83:LEU:O	1.61	1.16
1:D:85:HIS:CG	2:F:47:HIS:ND1	2.15	1.13
1:D:110:ASP:OD1	2:F:38:ARG:CZ	1.98	1.12
3:A:59:CYS:SG	3:A:66:CYS:CB	2.38	1.10
1:D:108:SER:O	1:D:112:ALA:HB2	1.51	1.08
1:C:83:ARG:NH1	2:E:49:PRO:O	1.86	1.08
1:D:85:HIS:CE1	2:F:47:HIS:CE1	2.44	1.05
1:D:110:ASP:OD1	2:F:38:ARG:NE	1.90	1.02
3:A:45:ASN:O	3:A:48:LEU:HG	1.58	1.02
1:D:85:HIS:HB2	2:F:47:HIS:HB3	1.41	1.01
1:D:110:ASP:OD1	2:F:38:ARG:NH2	1.94	1.01
1:D:103:SER:HB2	1:D:113:PHE:CE1	1.96	0.99
1:D:51:ALA:O	1:D:81:ARG:NH1	1.97	0.98
3:B:59:CYS:CB	3:B:66:CYS:SG	2.52	0.97
1:C:51:ALA:O	1:C:81:ARG:NH1	1.97	0.97
1:D:83:ARG:NH1	2:F:49:PRO:O	1.97	0.97
1:D:103:SER:HB2	1:D:113:PHE:CD1	2.05	0.92
1:D:111:THR:HG21	3:B:194:GLN:OE1	1.67	0.92
2:F:11:ALA:HB2	2:F:48:VAL:HG22	1.53	0.90
3:B:43:LEU:HD12	3:B:43:LEU:H	1.34	0.89
2:F:12:CYS:SG	2:F:46:TYR:CD2	2.65	0.89
1:D:103:SER:CB	1:D:113:PHE:CE1	2.55	0.89
3:B:59:CYS:SG	3:B:66:CYS:SG	1.02	0.88
1:D:85:HIS:ND1	2:F:47:HIS:ND1	2.21	0.87
2:E:11:ALA:HB2	2:E:48:VAL:HG22	1.55	0.87
1:D:111:THR:HG23	3:B:194:GLN:OE1	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:CYS:SG	2:F:46:TYR:HD2	1.98	0.86
1:D:85:HIS:CD2	2:F:47:HIS:ND1	2.43	0.85
2:F:12:CYS:HB3	2:F:46:TYR:HE2	1.43	0.83
1:C:296:LEU:HB3	1:C:299:LEU:HD12	1.62	0.82
2:F:12:CYS:HA	2:F:46:TYR:CD2	2.14	0.82
3:A:57:ASP:OD2	1:D:217:ARG:NH2	2.12	0.82
2:F:15:CYS:SG	2:F:42:ARG:HG3	2.20	0.82
3:A:57:ASP:CG	1:D:217:ARG:NH2	2.34	0.81
1:D:85:HIS:CE1	2:F:47:HIS:HE1	1.95	0.81
3:B:41:SER:OG	3:B:84:GLY:C	2.18	0.81
3:A:98:GLN:HA	3:A:121:LEU:HA	1.62	0.81
1:D:120:ARG:HA	1:D:144:ARG:HG3	1.62	0.81
3:B:40:PHE:CE2	3:B:83:LEU:HD13	2.16	0.80
3:A:440:ASN:HD22	3:A:442:PHE:HE2	1.29	0.80
1:C:120:ARG:HA	1:C:144:ARG:HG3	1.64	0.79
1:D:85:HIS:CE1	2:F:47:HIS:ND1	2.50	0.79
1:C:318:PRO:HG2	1:C:321:ALA:HB2	1.65	0.78
2:F:12:CYS:CB	2:F:46:TYR:CE2	2.66	0.78
3:A:44:VAL:O	3:A:48:LEU:HD23	1.84	0.78
1:D:296:LEU:HB3	1:D:299:LEU:HD12	1.66	0.78
2:E:15:CYS:SG	2:E:42:ARG:HB2	2.24	0.77
3:B:440:ASN:HD22	3:B:442:PHE:HE2	1.31	0.76
3:A:49:ASP:OD2	3:A:62:ARG:HG3	1.85	0.76
3:A:57:ASP:CG	1:D:217:ARG:HH21	1.88	0.76
1:D:318:PRO:HG2	1:D:321:ALA:HB2	1.67	0.76
3:B:98:GLN:HA	3:B:121:LEU:HA	1.66	0.76
3:A:482:MET:HG3	3:A:506:SER:HB2	1.67	0.75
1:C:256:LYS:HB2	3:A:186:LEU:HD11	1.67	0.75
1:D:402:ARG:NH1	3:B:89:PRO:HG3	2.02	0.75
3:A:56:SER:HB2	1:D:219:THR:HG21	1.68	0.74
3:A:56:SER:HB2	1:D:219:THR:CG2	2.18	0.74
3:B:433:ASP:HA	3:B:456:LEU:HA	1.69	0.74
1:C:157:GLY:HA2	1:C:181:LEU:HD23	1.69	0.74
3:B:482:MET:HG3	3:B:506:SER:HB2	1.69	0.73
3:B:403:ARG:HB3	3:B:425:GLU:HB3	1.71	0.73
2:F:23:ILE:HG13	2:F:38:ARG:HG3	1.71	0.73
3:B:533:VAL:HG11	3:B:538:LEU:HD11	1.70	0.72
2:F:12:CYS:HB3	2:F:46:TYR:CE2	2.24	0.72
2:F:11:ALA:HB2	2:F:48:VAL:CG2	2.20	0.72
3:A:433:ASP:HA	3:A:456:LEU:HA	1.71	0.72
3:B:188:TYR:HA	3:B:214:LEU:HD21	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:58:LEU:HD12	3:B:58:LEU:O	1.91	0.71
1:C:365:GLU:HG3	1:C:388:GLY:HA3	1.73	0.70
3:A:40:PHE:CE2	3:A:83:LEU:HD13	2.27	0.70
2:F:12:CYS:CB	2:F:46:TYR:HE2	2.02	0.70
3:A:45:ASN:HA	3:A:48:LEU:HD21	1.73	0.70
2:E:11:ALA:CB	2:E:48:VAL:HG22	2.21	0.69
1:D:103:SER:CB	1:D:113:PHE:CD1	2.72	0.69
2:F:39:CYS:O	2:F:46:TYR:N	2.19	0.69
1:D:85:HIS:NE2	2:F:47:HIS:CE1	2.61	0.69
2:F:11:ALA:CB	2:F:48:VAL:HG22	2.23	0.69
3:B:43:LEU:HD12	3:B:43:LEU:N	2.07	0.69
1:D:402:ARG:HH12	3:B:89:PRO:HG3	1.58	0.68
2:E:11:ALA:HB2	2:E:48:VAL:CG2	2.23	0.68
3:A:533:VAL:HG11	3:A:538:LEU:HD11	1.74	0.68
2:F:14:ALA:O	2:F:41:CYS:SG	2.52	0.68
3:A:403:ARG:HB3	3:A:425:GLU:HB3	1.76	0.68
2:F:12:CYS:SG	2:F:46:TYR:CE2	2.87	0.68
1:D:157:GLY:HA2	1:D:181:LEU:HD23	1.77	0.66
2:F:19:LYS:O	2:F:39:CYS:HA	1.94	0.66
3:A:57:ASP:OD1	1:D:217:ARG:NH2	2.27	0.65
3:A:311:PHE:HD1	3:A:335:ARG:HH11	1.41	0.65
1:D:365:GLU:HG3	1:D:388:GLY:HA3	1.78	0.65
2:F:23:ILE:O	2:F:35:VAL:HA	1.95	0.65
3:B:270:GLN:NE2	3:B:294:SER:OG	2.26	0.65
1:D:83:ARG:HH12	2:F:50:SER:HB2	1.61	0.64
2:E:40:THR:HB	2:E:45:TYR:HD1	1.62	0.64
3:A:270:GLN:NE2	3:A:294:SER:OG	2.25	0.64
3:B:305:ILE:O	3:B:308:ASN:ND2	2.30	0.64
1:C:105:GLY:O	1:C:113:PHE:HB2	1.97	0.63
3:A:522:LEU:O	3:A:524:ASN:N	2.32	0.63
1:C:365:GLU:OE2	1:C:365:GLU:N	2.32	0.63
1:D:107:LEU:HD23	3:B:194:GLN:HE22	1.64	0.63
2:F:23:ILE:HB	2:F:36:ILE:HG12	1.81	0.63
3:A:56:SER:HB3	1:D:239:LEU:HD12	1.80	0.62
1:C:190:HIS:ND1	1:C:214:SER:HB2	2.14	0.62
1:D:107:LEU:HD12	1:D:139:TYR:CD2	2.33	0.62
1:C:68:THR:OG1	1:C:116:CYS:SG	2.57	0.62
2:E:23:ILE:HB	2:E:36:ILE:HG12	1.80	0.62
1:C:141:CYS:O	1:C:168:ASN:ND2	2.32	0.62
1:C:85:HIS:HB2	2:E:47:HIS:HB3	1.82	0.62
1:D:214:SER:OG	1:D:234:ASP:OD1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:311:PHE:HD1	3:B:335:ARG:HH11	1.48	0.61
3:A:46:MET:O	3:A:62:ARG:NH2	2.33	0.61
1:D:256:LYS:HB2	3:B:186:LEU:HD11	1.81	0.61
2:F:11:ALA:CB	2:F:48:VAL:CG2	2.77	0.61
2:E:23:ILE:O	2:E:35:VAL:HA	1.99	0.61
1:D:190:HIS:CD2	1:D:191:LYS:HB2	2.35	0.61
1:D:190:HIS:ND1	1:D:214:SER:HB2	2.15	0.61
2:E:11:ALA:CB	2:E:48:VAL:CG2	2.79	0.61
2:E:12:CYS:SG	2:E:46:TYR:CD2	2.94	0.61
1:D:365:GLU:OE2	1:D:365:GLU:N	2.33	0.61
3:B:40:PHE:CD2	3:B:83:LEU:HD13	2.35	0.61
3:B:58:LEU:HD12	3:B:58:LEU:C	2.20	0.61
3:A:218:TRP:HB2	3:A:242:GLN:HG2	1.82	0.60
3:A:390:HIS:ND1	3:A:414:SER:OG	2.29	0.60
2:F:5:LEU:HD13	2:F:20:ARG:HH22	1.66	0.60
3:B:262:LEU:HB3	3:B:264:VAL:HG22	1.83	0.60
3:B:208:SER:O	3:B:211:MET:HB2	2.01	0.60
1:C:406:LEU:O	1:C:409:ASN:ND2	2.34	0.60
3:B:522:LEU:O	3:B:524:ASN:N	2.35	0.60
3:B:204:THR:HG22	3:B:205:GLY:H	1.67	0.59
1:D:141:CYS:O	1:D:168:ASN:ND2	2.31	0.59
3:B:61:TRP:O	3:B:64:VAL:HG22	2.03	0.59
3:B:218:TRP:HB2	3:B:242:GLN:HG2	1.84	0.59
1:C:214:SER:OG	1:C:234:ASP:OD1	2.21	0.59
1:C:232:VAL:HG23	1:C:256:LYS:HB3	1.85	0.59
1:C:287:ARG:NH2	3:B:57:ASP:OD2	2.35	0.59
3:A:305:ILE:O	3:A:308:ASN:ND2	2.31	0.59
1:C:85:HIS:CE1	2:E:47:HIS:ND1	2.71	0.58
1:C:83:ARG:HH12	2:E:50:SER:HB2	1.68	0.58
2:E:22:MET:SD	2:E:22:MET:N	2.76	0.58
1:D:68:THR:OG1	1:D:116:CYS:SG	2.60	0.58
3:A:43:LEU:N	3:A:43:LEU:HD12	2.18	0.58
3:A:192:VAL:O	3:A:194:GLN:NE2	2.34	0.58
3:A:262:LEU:HB3	3:A:264:VAL:HG22	1.85	0.58
1:D:82:GLY:HA3	2:F:10:TYR:HD1	1.69	0.58
2:E:5:LEU:HD13	2:E:20:ARG:HH22	1.69	0.57
3:B:33:LEU:O	3:B:50:TRP:HZ3	1.87	0.57
3:B:390:HIS:HB2	3:B:412:ASN:ND2	2.19	0.57
3:A:58:LEU:C	3:A:58:LEU:HD12	2.25	0.57
2:F:12:CYS:HA	2:F:46:TYR:CE2	2.39	0.57
1:C:190:HIS:CD2	1:C:191:LYS:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:514:LEU:HD12	3:B:514:LEU:H	1.70	0.56
3:B:41:SER:HB2	3:B:43:LEU:HD11	1.88	0.56
3:B:351:PRO:HG2	3:B:354:LEU:HD13	1.88	0.56
1:D:103:SER:HB2	1:D:113:PHE:HE1	1.58	0.56
3:A:188:TYR:CG	3:A:211:MET:HA	2.41	0.56
3:A:514:LEU:H	3:A:514:LEU:HD12	1.71	0.56
3:B:223:ARG:HB2	3:B:245:ASP:OD2	2.06	0.56
2:F:24:SER:HA	2:F:34:SER:O	2.06	0.56
1:D:179:GLY:O	1:D:204:ARG:NH1	2.39	0.55
3:A:219:TYR:HD1	3:A:243:ILE:HD12	1.71	0.55
3:A:188:TYR:HD1	3:A:214:LEU:HD11	1.71	0.55
3:A:68:ASN:HD22	1:D:146:PRO:HD2	1.71	0.55
3:A:390:HIS:HB2	3:A:412:ASN:ND2	2.21	0.55
1:D:167:GLU:HG2	1:D:191:LYS:HB3	1.89	0.55
3:B:228:THR:HG22	3:B:229:GLY:H	1.71	0.55
1:D:83:ARG:HH12	2:F:50:SER:CB	2.19	0.55
1:D:85:HIS:HA	2:F:49:PRO:HD3	1.89	0.55
3:A:40:PHE:CD2	3:A:83:LEU:HD13	2.41	0.55
3:A:68:ASN:ND2	1:D:146:PRO:HD2	2.21	0.55
3:B:222:VAL:HG21	3:B:227:LEU:HD11	1.88	0.55
1:C:70:ASN:ND2	1:C:114:PRO:HB2	2.22	0.54
2:E:12:CYS:SG	2:E:46:TYR:CE2	3.01	0.54
3:B:390:HIS:ND1	3:B:414:SER:OG	2.33	0.54
3:A:228:THR:HG22	3:A:229:GLY:H	1.72	0.54
3:B:41:SER:CB	3:B:83:LEU:O	2.55	0.54
3:A:204:THR:HG22	3:A:205:GLY:H	1.73	0.54
1:D:103:SER:HB3	1:D:113:PHE:CE1	2.42	0.54
1:D:232:VAL:HG23	1:D:256:LYS:HB3	1.89	0.54
2:F:22:MET:SD	2:F:22:MET:N	2.80	0.54
3:B:185:ARG:HA	3:B:188:TYR:CD2	2.43	0.54
1:D:396:THR:HG22	1:D:399:ARG:HH21	1.72	0.54
1:C:83:ARG:HH12	2:E:50:SER:CB	2.20	0.54
3:A:42:ASN:C	3:A:43:LEU:HD12	2.28	0.54
3:B:59:CYS:SG	3:B:66:CYS:HB2	2.38	0.54
1:C:83:ARG:O	2:E:48:VAL:HG13	2.08	0.54
3:B:219:TYR:HD1	3:B:243:ILE:HD12	1.72	0.53
3:A:222:VAL:HG21	3:A:227:LEU:HD11	1.90	0.53
1:D:194:LEU:N	1:D:216:ASN:OD1	2.40	0.53
1:C:390:VAL:HG11	1:C:406:LEU:HD13	1.91	0.53
3:A:59:CYS:SG	3:A:66:CYS:HB2	2.43	0.53
3:A:314:LYS:HG2	3:A:338:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:403:ARG:HB3	3:B:425:GLU:CB	2.39	0.53
1:C:139:TYR:HD1	1:C:166:ARG:HB3	1.72	0.53
1:D:406:LEU:O	1:D:409:ASN:ND2	2.38	0.53
3:A:185:ARG:HA	3:A:188:TYR:CD2	2.43	0.53
3:A:386:GLN:HG2	3:A:410:TYR:HB3	1.91	0.53
3:B:188:TYR:HA	3:B:214:LEU:CD2	2.39	0.53
3:B:403:ARG:HD3	3:B:425:GLU:HG2	1.91	0.53
1:D:208:LEU:HD21	1:D:211:LEU:HB2	1.91	0.52
2:F:12:CYS:CA	2:F:46:TYR:CE2	2.92	0.52
3:A:43:LEU:N	3:A:43:LEU:CD1	2.71	0.52
3:B:214:LEU:HD13	3:B:217:LEU:HD22	1.92	0.52
3:B:414:SER:HA	3:B:438:SER:O	2.09	0.52
2:F:16:SER:O	2:F:18:CYS:N	2.42	0.52
3:A:219:TYR:CE2	3:A:221:ASP:HB2	2.44	0.52
1:D:139:TYR:HD1	1:D:166:ARG:HB3	1.73	0.52
3:B:437:LEU:HB2	3:B:461:LEU:HD23	1.92	0.52
1:C:194:LEU:N	1:C:216:ASN:OD1	2.42	0.52
1:D:281:LEU:HD23	1:D:305:LEU:HD13	1.92	0.52
3:B:294:SER:HB2	3:B:318:HIS:CD2	2.45	0.52
1:C:52:ARG:HH11	1:C:81:ARG:NH2	2.08	0.52
3:A:45:ASN:O	3:A:48:LEU:CG	2.46	0.52
3:B:219:TYR:CE2	3:B:221:ASP:HB2	2.44	0.52
3:B:314:LYS:HG2	3:B:338:TYR:HB2	1.91	0.52
3:A:414:SER:HA	3:A:438:SER:O	2.10	0.51
1:C:167:GLU:HG2	1:C:191:LYS:HB3	1.92	0.51
3:B:266:THR:OG1	2:F:35:VAL:O	2.29	0.51
3:B:461:LEU:HB2	3:B:485:VAL:HG12	1.92	0.51
3:A:223:ARG:HG3	3:A:247:SER:O	2.11	0.51
3:A:451:GLY:HA3	3:A:473:GLU:HB3	1.93	0.51
1:C:291:PRO:HA	1:C:315:THR:HG21	1.92	0.51
2:E:16:SER:O	2:E:18:CYS:N	2.44	0.51
3:A:270:GLN:HE21	3:A:294:SER:HG	1.55	0.51
3:A:79:SER:HB2	3:A:103:GLN:HG2	1.92	0.51
1:C:280:LEU:HD12	1:C:304:ALA:HB3	1.92	0.51
1:D:82:GLY:HA3	2:F:10:TYR:CD1	2.46	0.51
1:D:179:GLY:HA3	1:D:201:SER:HB2	1.93	0.51
2:E:25:PHE:HE2	2:E:36:ILE:HG23	1.76	0.51
3:A:323:THR:HG22	3:A:345:LYS:HB2	1.93	0.50
3:A:437:LEU:HB2	3:A:461:LEU:HD23	1.93	0.50
3:B:36:ILE:HA	3:B:88:SER:HB3	1.93	0.50
3:B:223:ARG:HG3	3:B:247:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:386:GLN:HG2	3:B:410:TYR:HB3	1.93	0.50
2:F:12:CYS:CA	2:F:46:TYR:CD2	2.89	0.50
3:A:274:LEU:HD12	3:A:296:ASN:ND2	2.27	0.50
1:D:52:ARG:HH11	1:D:81:ARG:NH2	2.08	0.50
1:C:82:GLY:HA3	2:E:10:TYR:HD1	1.76	0.50
3:A:333:MET:O	3:A:335:ARG:N	2.45	0.50
1:C:57:GLU:OE2	1:C:98:HIS:ND1	2.42	0.50
3:B:37:LYS:NZ	3:B:50:TRP:O	2.42	0.50
3:B:451:GLY:HA3	3:B:473:GLU:HB3	1.94	0.50
1:D:83:ARG:NH1	2:F:50:SER:HB2	2.27	0.50
1:C:83:ARG:NH1	2:E:50:SER:HB2	2.27	0.50
3:A:50:TRP:CD1	3:A:50:TRP:N	2.79	0.50
3:A:292:ASP:OD1	3:A:316:TYR:HB2	2.12	0.50
1:D:291:PRO:HA	1:D:315:THR:HG21	1.94	0.50
3:A:164:THR:HG21	3:A:186:LEU:HG	1.94	0.49
1:C:179:GLY:HA3	1:C:201:SER:HB2	1.94	0.49
3:B:239:THR:OG1	2:F:51:ARG:HG3	2.11	0.49
3:A:45:ASN:HA	3:A:48:LEU:CD2	2.40	0.49
2:F:12:CYS:CB	2:F:46:TYR:CD2	2.95	0.49
3:B:185:ARG:HA	3:B:188:TYR:HD2	1.77	0.49
3:A:512:ASN:HB3	3:A:514:LEU:HD12	1.95	0.49
1:D:54:GLU:HG2	1:D:57:GLU:HG3	1.94	0.49
2:E:40:THR:HB	2:E:45:TYR:CD1	2.45	0.49
3:B:292:ASP:OD1	3:B:316:TYR:HB2	2.12	0.49
2:F:25:PHE:HE2	2:F:36:ILE:HG23	1.77	0.49
3:A:188:TYR:CD1	3:A:211:MET:HA	2.48	0.49
3:A:294:SER:HB2	3:A:318:HIS:CD2	2.48	0.49
1:D:85:HIS:HB2	2:F:47:HIS:CB	2.27	0.49
1:C:85:HIS:HA	2:E:49:PRO:HD3	1.95	0.49
1:C:297:GLN:OE1	1:C:297:GLN:N	2.46	0.49
3:A:82:ASN:HA	3:A:105:ASN:HA	1.95	0.48
3:A:351:PRO:HG2	3:A:354:LEU:HD13	1.93	0.48
1:D:390:VAL:HG11	1:D:406:LEU:HD13	1.95	0.48
1:C:100:VAL:HG13	1:C:134:LYS:HB2	1.95	0.48
1:C:281:LEU:HD23	1:C:305:LEU:HD13	1.95	0.48
2:E:15:CYS:O	2:E:41:CYS:SG	2.71	0.48
3:B:149:ASN:HA	3:B:173:ASP:OD1	2.13	0.48
2:E:39:CYS:O	2:E:45:TYR:HA	2.12	0.48
1:C:354:VAL:HG13	1:C:378:GLU:HB2	1.95	0.48
3:A:218:TRP:HB2	3:A:242:GLN:CG	2.42	0.48
1:D:65:MET:SD	1:D:104:PHE:HE1	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:164:THR:HG21	3:B:186:LEU:HG	1.94	0.48
3:B:323:THR:HG22	3:B:345:LYS:HB2	1.96	0.48
3:B:91:ILE:HD11	3:B:100:ILE:HD13	1.96	0.48
1:D:255:ILE:HA	1:D:278:LEU:HA	1.95	0.48
3:B:283:GLY:HA3	3:B:305:ILE:HG12	1.94	0.48
1:C:278:LEU:HD21	1:C:281:LEU:HB2	1.94	0.48
1:C:400:MET:SD	1:C:404:LEU:HB2	2.54	0.48
3:B:218:TRP:HB2	3:B:242:GLN:CG	2.43	0.48
1:D:400:MET:SD	1:D:404:LEU:HB2	2.54	0.48
3:B:192:VAL:O	3:B:194:GLN:NE2	2.35	0.48
3:A:223:ARG:HB2	3:A:245:ASP:OD2	2.14	0.47
2:F:12:CYS:SG	2:F:41:CYS:HB2	2.54	0.47
1:C:179:GLY:O	1:C:204:ARG:NH1	2.48	0.47
3:A:279:PRO:HB2	3:A:282:ILE:HG13	1.96	0.47
3:B:82:ASN:HA	3:B:105:ASN:HA	1.95	0.47
1:C:87:ILE:HA	1:C:101:SER:O	2.14	0.47
1:D:65:MET:O	1:D:68:THR:HG22	2.14	0.47
1:D:85:HIS:NE2	2:F:47:HIS:ND1	2.62	0.47
1:D:297:GLN:N	1:D:297:GLN:OE1	2.47	0.47
3:A:36:ILE:HA	3:A:88:SER:HB3	1.97	0.47
1:D:230:LEU:HD23	1:D:254:LEU:HD21	1.97	0.47
3:A:403:ARG:HB3	3:A:425:GLU:CB	2.44	0.47
1:D:100:VAL:HG13	1:D:134:LYS:HB2	1.96	0.47
1:C:238:ASN:O	1:C:262:ASN:HA	2.15	0.47
2:E:5:LEU:HD11	3:A:311:PHE:CG	2.50	0.47
3:B:238:CYS:HB2	3:B:262:LEU:HD21	1.96	0.47
3:B:512:ASN:HB3	3:B:514:LEU:HD12	1.97	0.47
3:A:50:TRP:CD1	3:A:61:TRP:HB3	2.50	0.47
3:A:58:LEU:O	3:A:64:VAL:HG21	2.14	0.47
2:F:16:SER:N	2:F:17:PRO:HD2	2.30	0.47
3:A:518:ILE:HG13	3:A:538:LEU:HD13	1.98	0.47
3:A:504:LEU:HD21	3:A:507:LEU:HB2	1.97	0.46
2:E:51:ARG:HG3	3:A:239:THR:HG21	1.96	0.46
3:A:185:ARG:HA	3:A:188:TYR:HD2	1.80	0.46
1:D:62:TYR:CE2	1:D:74:ALA:HA	2.51	0.46
3:B:504:LEU:HD21	3:B:507:LEU:HB2	1.97	0.46
1:C:255:ILE:HA	1:C:278:LEU:HA	1.97	0.46
3:B:41:SER:HB2	3:B:43:LEU:CD1	2.45	0.46
1:C:402:ARG:NH1	3:A:89:PRO:HG3	2.30	0.46
1:D:184:LEU:HD21	1:D:187:LEU:HD13	1.98	0.46
3:B:50:TRP:N	3:B:50:TRP:CD1	2.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:190:ASN:O	3:B:214:LEU:HA	2.16	0.46
1:C:333:LEU:HB2	1:C:357:LEU:HD23	1.98	0.46
2:E:12:CYS:SG	2:E:46:TYR:HD2	2.36	0.46
3:A:283:GLY:O	3:A:308:ASN:ND2	2.42	0.46
3:A:311:PHE:HD1	3:A:335:ARG:NH1	2.11	0.46
1:C:230:LEU:HD23	1:C:254:LEU:HD21	1.98	0.46
1:D:103:SER:HB2	1:D:113:PHE:HD1	1.74	0.46
3:B:41:SER:OG	3:B:84:GLY:O	2.33	0.46
3:B:333:MET:O	3:B:335:ARG:N	2.49	0.46
3:A:91:ILE:HD11	3:A:100:ILE:HD13	1.97	0.46
3:A:283:GLY:HA3	3:A:305:ILE:HG12	1.97	0.46
3:A:149:ASN:HA	3:A:173:ASP:OD1	2.15	0.46
3:B:379:SER:HA	3:B:405:LEU:HD21	1.98	0.46
1:C:82:GLY:HA3	2:E:10:TYR:CD1	2.50	0.46
3:B:531:LEU:HD11	3:B:533:VAL:HG23	1.98	0.46
3:A:247:SER:HB3	3:A:270:GLN:H	1.81	0.45
3:A:278:ILE:HD13	3:A:293:LEU:HD12	1.98	0.45
3:A:504:LEU:O	3:A:527:THR:OG1	2.31	0.45
3:B:309:LEU:HD23	3:B:312:THR:HG21	1.98	0.45
1:C:65:MET:O	1:C:68:THR:HG22	2.17	0.45
1:D:85:HIS:CD2	2:F:47:HIS:CE1	3.03	0.45
1:C:202:PHE:HB3	1:C:225:PHE:CZ	2.52	0.45
2:E:38:ARG:HD3	2:E:45:TYR:CD2	2.52	0.45
3:A:311:PHE:CD1	3:A:335:ARG:NH1	2.85	0.45
1:C:62:TYR:CE2	1:C:74:ALA:HA	2.52	0.45
1:C:85:HIS:HB2	2:E:47:HIS:CB	2.46	0.45
1:D:139:TYR:CD1	1:D:166:ARG:HB3	2.50	0.45
3:A:56:SER:HB3	1:D:239:LEU:CD1	2.45	0.45
3:A:247:SER:HB3	3:A:270:GLN:N	2.32	0.45
1:D:83:ARG:O	2:F:48:VAL:HG13	2.16	0.45
3:B:79:SER:HB2	3:B:103:GLN:HG2	1.98	0.45
2:E:39:CYS:O	2:E:46:TYR:N	2.44	0.44
1:D:88:GLU:CD	2:F:51:ARG:HB2	2.38	0.44
3:B:274:LEU:HD12	3:B:296:ASN:ND2	2.32	0.44
1:D:280:LEU:HD12	1:D:304:ALA:HB3	1.99	0.44
1:D:333:LEU:HB2	1:D:357:LEU:HD23	1.99	0.44
1:D:171:LEU:HA	1:D:171:LEU:HD23	1.72	0.44
1:C:184:LEU:HD21	1:C:187:LEU:HD13	1.98	0.44
1:D:70:ASN:HB3	1:D:72:TRP:NE1	2.32	0.44
3:B:363:LEU:HD11	3:B:365:LEU:HD21	1.99	0.44
3:B:429:ILE:HB	3:B:432:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:247:SER:HB3	3:B:270:GLN:H	1.82	0.44
1:C:70:ASN:HB3	1:C:72:TRP:NE1	2.33	0.44
3:A:388:ASN:HD22	3:A:410:TYR:HE2	1.66	0.44
3:B:504:LEU:O	3:B:527:THR:OG1	2.34	0.44
1:C:139:TYR:CD1	1:C:166:ARG:HB3	2.51	0.44
1:C:273:ASN:ND2	1:C:296:LEU:HA	2.33	0.44
3:A:342:ASN:OD1	3:A:364:ASN:ND2	2.51	0.44
1:D:87:ILE:HA	1:D:101:SER:O	2.18	0.44
3:B:109:GLY:HA2	3:B:132:TYR:CZ	2.53	0.44
3:B:270:GLN:HE21	3:B:294:SER:HG	1.61	0.44
1:C:278:LEU:HD23	1:C:302:LEU:HD13	2.00	0.44
3:A:429:ILE:HB	3:A:432:LEU:HD12	1.99	0.44
3:B:480:ILE:HG21	3:B:501:LEU:HD13	1.99	0.44
3:A:147:THR:HG23	3:A:171:ARG:HB3	2.00	0.44
1:D:90:MET:HG2	1:D:100:VAL:HG21	2.00	0.44
3:B:87:ILE:HG12	3:B:107:LEU:HD13	1.99	0.44
2:E:35:VAL:O	3:A:266:THR:OG1	2.36	0.43
1:D:59:ASP:HA	1:D:62:TYR:HD1	1.81	0.43
3:B:278:ILE:HD13	3:B:293:LEU:HD12	2.00	0.43
1:D:57:GLU:OE2	1:D:98:HIS:ND1	2.47	0.43
3:B:311:PHE:HD1	3:B:335:ARG:NH1	2.14	0.43
3:A:169:LEU:HD21	3:A:172:LEU:HB2	1.99	0.43
3:A:357:LEU:HD12	3:A:360:LEU:HD22	2.00	0.43
3:A:490:LEU:HD12	3:A:512:ASN:HD21	1.83	0.43
3:B:279:PRO:HB2	3:B:282:ILE:HG13	1.99	0.43
3:B:518:ILE:HG13	3:B:538:LEU:HD13	1.99	0.43
1:C:54:GLU:HG2	1:C:57:GLU:HG3	2.01	0.43
3:A:245:ASP:OD2	3:A:247:SER:OG	2.35	0.43
3:A:238:CYS:HB2	3:A:262:LEU:HD21	2.01	0.43
3:B:247:SER:HB3	3:B:270:GLN:N	2.33	0.43
1:C:397:VAL:O	1:C:397:VAL:HG12	2.18	0.43
3:A:64:VAL:HG12	3:A:76:LEU:HD13	2.00	0.43
3:A:327:PRO:HB2	3:A:330:LEU:HD13	2.00	0.43
3:B:255:ILE:HG12	3:B:274:LEU:HD22	2.01	0.43
3:B:296:ASN:O	3:B:320:ASN:HA	2.19	0.43
2:F:15:CYS:C	2:F:17:PRO:HD2	2.39	0.43
3:B:506:SER:HA	3:B:530:ASN:O	2.19	0.43
1:D:58:GLN:HG2	1:D:62:TYR:CE1	2.54	0.42
2:F:5:LEU:HD13	2:F:20:ARG:NH2	2.31	0.42
1:D:238:ASN:O	1:D:262:ASN:HA	2.18	0.42
3:B:277:ARG:HG2	3:B:300:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:311:PHE:CG	2:F:5:LEU:HD11	2.54	0.42
3:A:531:LEU:HD11	3:A:533:VAL:HG23	2.01	0.42
1:D:85:HIS:O	1:D:114:PRO:HD3	2.19	0.42
3:B:327:PRO:HB2	3:B:330:LEU:HD13	2.02	0.42
1:D:52:ARG:HA	1:D:52:ARG:HD3	1.62	0.42
3:A:127:SER:HB2	3:A:151:LYS:HB3	2.01	0.42
1:C:90:MET:HG2	1:C:100:VAL:HG21	2.01	0.42
1:C:156:LEU:HD13	1:C:160:LEU:HD13	2.02	0.42
1:C:205:PHE:O	1:C:227:LEU:HD22	2.20	0.42
3:A:68:ASN:OD1	3:A:68:ASN:N	2.51	0.42
1:D:374:LYS:O	1:D:399:ARG:NH2	2.53	0.42
3:B:43:LEU:N	3:B:43:LEU:CD1	2.73	0.42
3:B:239:THR:HG21	2:F:51:ARG:HA	2.01	0.42
3:A:252:THR:HA	3:A:273:ARG:O	2.20	0.41
3:A:536:ASN:HD22	3:A:536:ASN:HA	1.64	0.41
3:B:32:ALA:O	3:B:36:ILE:HG13	2.20	0.41
3:B:169:LEU:HD21	3:B:172:LEU:HB2	2.00	0.41
1:C:328:LEU:HD12	1:C:329:MET:N	2.35	0.41
1:D:88:GLU:OE2	2:F:51:ARG:HB2	2.20	0.41
1:D:278:LEU:HD21	1:D:281:LEU:HB2	2.02	0.41
1:C:59:ASP:HA	1:C:62:TYR:HD1	1.83	0.41
1:C:304:ALA:HB1	1:C:306:MET:CE	2.50	0.41
3:A:381:CYS:HB2	3:A:384:LEU:HB2	2.02	0.41
1:D:273:ASN:ND2	1:D:296:LEU:HA	2.35	0.41
1:C:58:GLN:HG2	1:C:62:TYR:CE1	2.54	0.41
1:C:110:ASP:HA	1:C:111:THR:HA	1.83	0.41
3:A:41:SER:OG	3:A:43:LEU:HD13	2.21	0.41
3:A:403:ARG:HD3	3:A:425:GLU:HG2	2.02	0.41
1:D:398:TRP:O	1:D:401:ARG:HG3	2.20	0.41
3:B:311:PHE:CD1	2:F:5:LEU:HD11	2.55	0.41
1:C:88:GLU:OE2	2:E:51:ARG:HB2	2.20	0.41
1:C:310:ASN:HB2	1:C:336:THR:HG22	2.02	0.41
3:A:254:GLU:OE1	3:A:254:GLU:N	2.39	0.41
1:D:354:VAL:HG13	1:D:378:GLU:HB2	2.02	0.41
3:A:80:SER:N	3:A:103:GLN:O	2.38	0.41
3:A:111:ILE:HG12	3:A:131:LEU:HD13	2.02	0.41
1:D:85:HIS:CB	2:F:47:HIS:HB3	2.31	0.41
1:D:202:PHE:HB3	1:D:225:PHE:CZ	2.55	0.41
1:C:138:PHE:HB2	1:C:165:LEU:HD23	2.02	0.41
1:C:189:LEU:HD12	1:C:213:LEU:HD21	2.03	0.41
1:C:208:LEU:HD21	1:C:211:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ALA:HB1	1:D:306:MET:CE	2.51	0.41
3:B:135:ILE:HA	3:B:136:PRO:HD3	1.94	0.41
1:C:249:THR:HA	1:C:275:LEU:HD21	2.03	0.41
3:A:345:LYS:HG2	3:A:369:ARG:NH1	2.36	0.41
3:A:461:LEU:HB2	3:A:485:VAL:HG12	2.02	0.41
1:D:205:PHE:O	1:D:227:LEU:HD22	2.20	0.41
1:D:280:LEU:HD21	3:B:165:GLN:HE21	1.86	0.41
3:B:171:ARG:HG3	3:B:195:TYR:HB3	2.02	0.41
3:B:269:LEU:O	3:B:296:ASN:ND2	2.54	0.41
3:B:311:PHE:CD1	3:B:335:ARG:NH1	2.89	0.41
3:B:440:ASN:O	3:B:464:ASN:HA	2.20	0.41
1:C:218:LEU:HB3	1:C:240:LEU:HD21	2.03	0.41
3:B:199:ARG:HD3	3:B:221:ASP:OD2	2.20	0.41
3:A:328:SER:HB2	3:A:353:GLU:OE1	2.21	0.40
3:B:199:ARG:HA	3:B:223:ARG:O	2.22	0.40
3:B:508:ILE:HG23	3:B:532:ASN:HB3	2.03	0.40
1:C:54:GLU:HA	1:C:55:PRO:HD3	1.95	0.40
3:A:87:ILE:HG12	3:A:107:LEU:HD13	2.02	0.40
3:A:440:ASN:O	3:A:464:ASN:HA	2.21	0.40
1:D:107:LEU:HD12	1:D:107:LEU:HA	1.93	0.40
1:D:111:THR:HG22	3:B:194:GLN:OE1	2.02	0.40
1:D:249:THR:HA	1:D:275:LEU:HD21	2.03	0.40
3:B:345:LYS:HG2	3:B:369:ARG:NH1	2.36	0.40
1:D:88:GLU:HB2	1:D:101:SER:HB3	2.03	0.40
3:B:206:THR:HG23	3:B:229:GLY:HA3	2.03	0.40
3:A:296:ASN:O	3:A:320:ASN:HA	2.20	0.40
3:B:283:GLY:O	3:B:308:ASN:ND2	2.46	0.40
3:B:512:ASN:H	3:B:536:ASN:ND2	2.19	0.40
1:C:85:HIS:CD2	2:E:47:HIS:ND1	2.90	0.40
1:C:172:GLY:O	1:C:194:LEU:HA	2.22	0.40
3:A:419:LYS:HG2	3:A:441:ASN:HB2	2.04	0.40
3:A:527:THR:O	3:A:529:VAL:HG23	2.22	0.40
3:B:357:LEU:HD12	3:B:360:LEU:HD22	2.04	0.40

All (3) 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)
1:D:326:LYS:NZ	3:B:404:ASN:O[1_655]	1.86	0.34
1:C:326:LYS:NZ	3:A:404:ASN:O[1_545]	1.89	0.31
2:E:42:ARG:NH1	3:B:54:HIS:NE2[1_565]	2.11	0.09

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	C	361/433 (83%)	316 (88%)	41 (11%)	4 (1%)	14 50
1	D	361/433 (83%)	317 (88%)	41 (11%)	3 (1%)	19 57
2	E	41/52 (79%)	32 (78%)	5 (12%)	4 (10%)	0 6
2	F	41/52 (79%)	32 (78%)	5 (12%)	4 (10%)	0 6
3	A	509/555 (92%)	439 (86%)	68 (13%)	2 (0%)	34 70
3	B	509/555 (92%)	437 (86%)	71 (14%)	1 (0%)	47 80
All	All	1822/2080 (88%)	1573 (86%)	231 (13%)	18 (1%)	15 52

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	49	PRO
2	F	49	PRO
3	A	50	TRP
3	A	334	SER
3	B	334	SER
1	C	391	PRO
1	D	391	PRO
2	F	17	PRO
2	F	47	HIS
1	C	108	SER
2	F	48	VAL
2	E	47	HIS
2	E	48	VAL
2	E	17	PRO
1	C	146	PRO
1	C	243	PRO
1	D	146	PRO
1	D	243	PRO

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	C	320/378 (85%)	312 (98%)	8 (2%)	47 74
1	D	320/378 (85%)	312 (98%)	8 (2%)	47 74
2	E	39/45 (87%)	33 (85%)	6 (15%)	2 14
2	F	39/45 (87%)	33 (85%)	6 (15%)	2 14
3	A	450/485 (93%)	441 (98%)	9 (2%)	55 79
3	B	450/485 (93%)	434 (96%)	16 (4%)	35 65
All	All	1618/1816 (89%)	1565 (97%)	53 (3%)	38 68

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	ARG
1	C	78	ASP
1	C	203	ASN
1	C	280	LEU
1	C	292	PHE
1	C	296	LEU
1	C	394	ARG
1	C	396	THR
2	E	8	CYS
2	E	15	CYS
2	E	22	MET
2	E	41	CYS
2	E	47	HIS
2	E	49	PRO
3	A	40	PHE
3	A	49	ASP
3	A	67	ASP
3	A	128	GLU
3	A	212	CYS
3	A	214	LEU
3	A	308	ASN
3	A	440	ASN

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Mol	Chain	Res	Type
3	A	514	LEU
1	D	52	ARG
1	D	78	ASP
1	D	107	LEU
1	D	111	THR
1	D	125	GLU
1	D	203	ASN
1	D	292	PHE
1	D	296	LEU
3	B	40	PHE
3	B	41	SER
3	B	43	LEU
3	B	48	LEU
3	B	51	ASP
3	B	54	HIS
3	B	56	SER
3	B	58	LEU
3	B	67	ASP
3	B	128	GLU
3	B	211	MET
3	B	212	CYS
3	B	213	GLN
3	B	214	LEU
3	B	308	ASN
3	B	514	LEU
2	F	8	CYS
2	F	15	CYS
2	F	22	MET
2	F	44	ARG
2	F	47	HIS
2	F	49	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	364	ASN
3	A	536	ASN
1	D	85	HIS
3	B	511	ASN
3	B	536	ASN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	C	363/433 (83%)	0.32	14 (3%)	39	36	41, 56, 75, 85	0
1	D	363/433 (83%)	0.40	17 (4%)	31	30	40, 58, 74, 86	0
2	E	45/52 (86%)	0.78	5 (11%)	5	7	51, 72, 94, 99	0
2	F	45/52 (86%)	0.73	7 (15%)	2	3	51, 74, 96, 103	0
3	A	513/555 (92%)	0.43	44 (8%)	10	12	36, 49, 60, 76	0
3	B	513/555 (92%)	0.53	48 (9%)	8	10	40, 52, 83, 102	0
All	All	1842/2080 (88%)	0.45	135 (7%)	15	16	36, 53, 77, 103	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	143	GLY	6.6
3	B	75	SER	6.0
1	D	144	ARG	5.2
3	B	47	LEU	5.1
3	B	63	GLY	4.9
1	D	142	LEU	4.8
1	C	84	TRP	4.2
3	A	265	ALA	4.1
3	B	90	ALA	4.1
1	D	53	THR	4.0
3	B	33	LEU	4.0
3	A	40	PHE	3.8
3	A	255	ILE	3.8
1	D	82	GLY	3.8
3	B	91	ILE	3.7
3	A	461	LEU	3.7
1	C	343	PRO	3.7
3	B	255	ILE	3.6
3	A	485	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
3	B	76	LEU	3.6
3	B	65	PHE	3.5
1	D	84	TRP	3.5
3	A	254	GLU	3.5
3	B	470	LEU	3.5
3	A	470	LEU	3.5
3	A	508	ILE	3.4
2	E	5	LEU	3.4
3	A	447	PRO	3.3
3	A	46	MET	3.3
1	D	79	VAL	3.3
3	A	64	VAL	3.3
3	A	47	LEU	3.2
3	B	531	LEU	3.1
3	A	49	ASP	3.1
1	C	390	VAL	3.1
3	A	532	ASN	3.1
3	B	77	ASN	3.1
3	B	273	ARG	3.1
3	A	495	PRO	3.1
3	A	446	ILE	3.1
3	B	485	VAL	3.1
3	A	531	LEU	3.0
3	A	317	LEU	3.0
3	A	75	SER	3.0
2	F	19	LYS	3.0
3	B	54	HIS	3.0
1	C	73	ALA	3.0
1	D	217	ARG	2.9
2	E	15	CYS	2.9
3	B	87	ILE	2.9
3	B	471	PRO	2.9
1	C	392	PHE	2.9
1	D	50	GLY	2.9
1	C	50	GLY	2.8
3	A	448	LEU	2.8
3	B	446	ILE	2.8
1	C	391	PRO	2.8
2	E	14	ALA	2.7
3	B	461	LEU	2.7
1	C	51	ALA	2.7
3	B	507	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	471	PRO	2.7
3	A	78	LEU	2.7
2	F	4	SER	2.7
1	C	71	ASP	2.7
3	B	71	TYR	2.6
1	D	412	LEU	2.6
3	B	365	LEU	2.6
3	B	488	ASN	2.6
3	B	254	GLU	2.6
3	B	78	LEU	2.6
3	B	474	PHE	2.6
1	C	355	LEU	2.6
3	A	494	ILE	2.6
3	A	484	ASP	2.5
1	C	292	PHE	2.5
2	E	6	PRO	2.5
3	B	465	HIS	2.5
2	F	21	VAL	2.5
3	B	38	GLY	2.5
3	B	364	ASN	2.5
3	B	526	PHE	2.5
3	A	522	LEU	2.5
1	D	61	VAL	2.4
3	B	469	GLN	2.4
3	B	62	ARG	2.4
3	B	478	ARG	2.4
3	B	46	MET	2.4
3	A	287	ALA	2.4
3	B	489	LEU	2.4
2	F	5	LEU	2.4
1	C	82	GLY	2.4
1	D	390	VAL	2.4
3	A	87	ILE	2.3
3	B	32	ALA	2.3
3	A	266	THR	2.3
3	A	62	ARG	2.3
3	B	533	VAL	2.3
3	B	426	LEU	2.3
1	D	57	GLU	2.3
3	B	411	LEU	2.3
3	A	488	ASN	2.3
2	F	6	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	342	ILE	2.2
3	B	88	SER	2.2
3	A	298	LEU	2.2
3	A	363	LEU	2.2
3	B	448	LEU	2.2
3	A	54	HIS	2.2
1	D	366	ILE	2.2
3	A	44	VAL	2.2
3	B	281	VAL	2.2
3	B	191	GLU	2.2
3	B	279	PRO	2.2
2	E	52	ALA	2.2
3	A	464	ASN	2.2
3	A	507	LEU	2.2
2	F	37	TYR	2.2
3	A	533	VAL	2.2
3	A	63	GLY	2.2
1	D	110	ASP	2.2
3	B	74	VAL	2.1
1	D	128	THR	2.1
1	C	379	LEU	2.1
3	A	354	LEU	2.1
3	A	48	LEU	2.1
3	A	77	ASN	2.1
3	B	36	ILE	2.1
3	B	94	LEU	2.1
2	F	52	ALA	2.1
3	A	86	GLU	2.1
3	A	55	ASN	2.1
3	B	495	PRO	2.0
3	A	483	ILE	2.0
1	D	127	LEU	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.