



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:18 AM UTC

PDB ID : 5XKJ / pdb_00005xkj
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	:	4-5-2 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

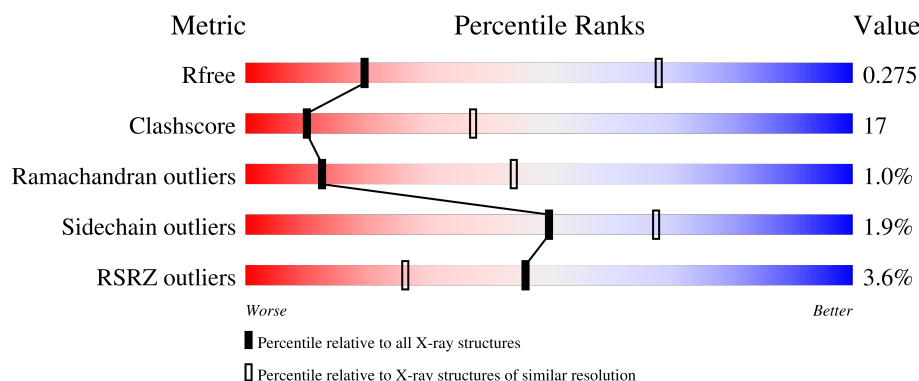
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	C	433	
1	D	433	
2	E	52	
2	F	52	
3	A	555	

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Mol	Chain	Length	Quality of chain
3	B	555	4% 64% 27% 8%

2 Entry composition

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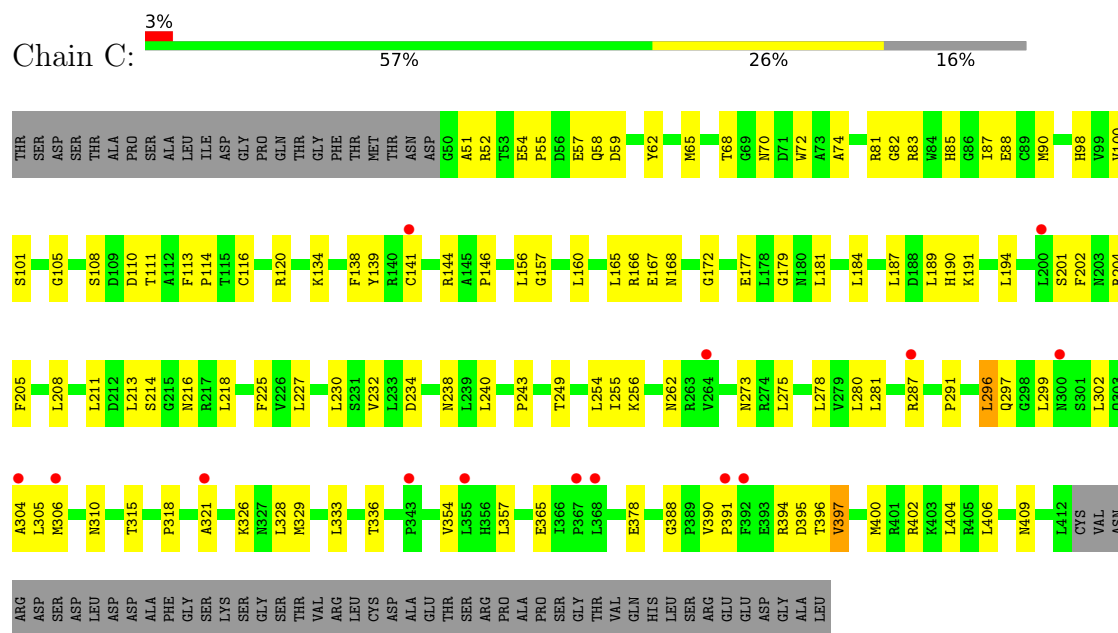
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Chain	Residue	Modelled	Actual	Comment	Reference
B	575	HIS	-	expression tag	UNP C0LGW6
B	576	HIS	-	expression tag	UNP C0LGW6
B	577	HIS	-	expression tag	UNP C0LGW6
B	578	HIS	-	expression tag	UNP C0LGW6

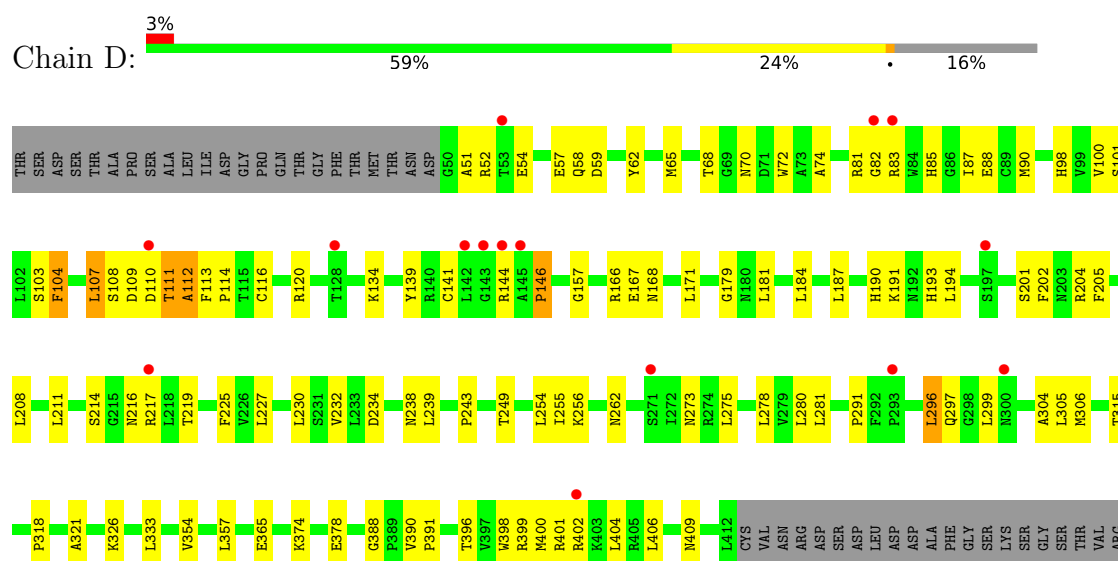
3 Residue-property plots

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

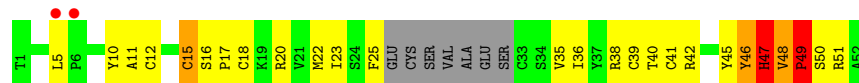


• Molecule 1: Protein TOO MANY MOUTHS

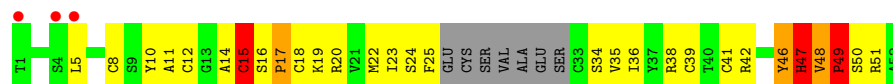


LEU
CYS
ASP
ALA
GLU
THR
SER
ARG
PRO
ALA
PRO
SER
GLY
THR
VAL
GLN
HIS
LEU
SER
ARG
GLU
GLU
ASP
GLY
ALA
LEU

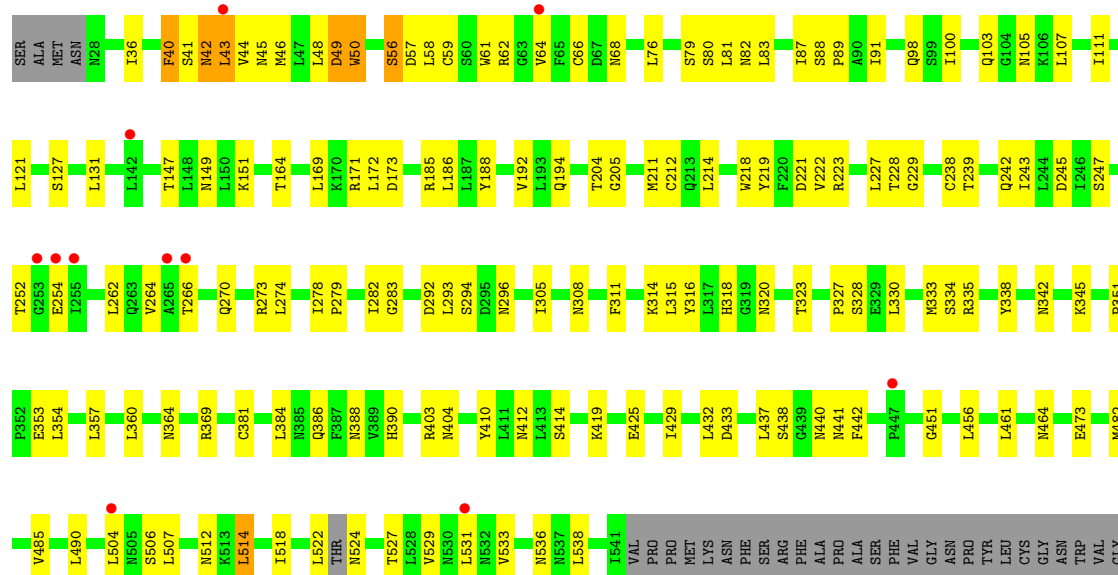
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 2



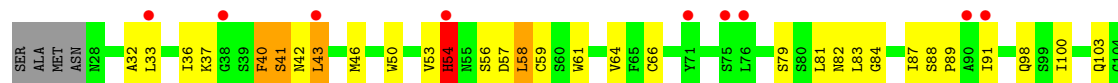
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 2

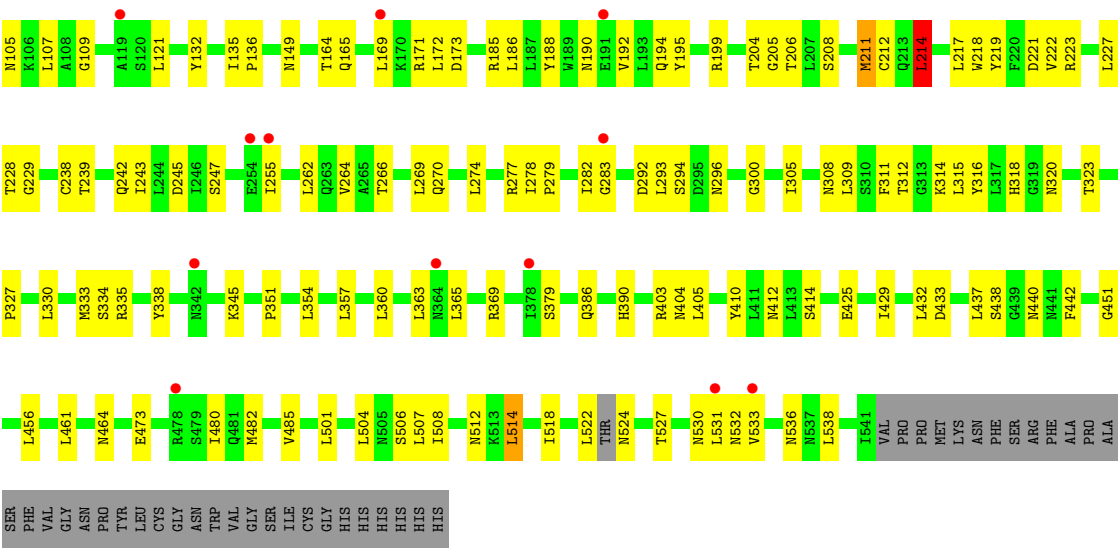


• Molecule 3: LRR receptor-like serine/threonine-protein kinase ERL1



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





4 Data and refinement statistics

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 46.19 – 3.48	Depositor EDS
% Data completeness (in resolution range)	94.7 (46.19-3.48) 94.7 (46.19-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.254 , 0.277 0.255 , 0.275	Depositor DCC
R_{free} test set	1420 reflections (4.79%)	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)	0.32 , 13.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	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.*

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	C	0.28	0/2883	0.52	2/3915 (0.1%)
1	D	0.30	0/2883	0.58	5/3915 (0.1%)
2	E	0.59	0/347	1.10	2/466 (0.4%)
2	F	0.60	0/347	1.02	3/466 (0.6%)
3	A	0.32	0/3985	0.49	2/5419 (0.0%)
3	B	0.32	0/3985	0.53	3/5419 (0.1%)
All	All	0.32	0/14430	0.57	17/19600 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	104	PHE	CA-C-N	-8.22	115.08	122.73
1	D	104	PHE	C-N-CA	-8.22	115.08	122.73
3	B	214	LEU	N-CA-C	-7.84	92.17	107.62
1	D	109	ASP	N-CA-C	7.42	121.60	112.54
2	E	49	PRO	CB-CA-C	-7.31	99.49	111.56
2	E	46	TYR	N-CA-C	7.00	118.63	108.34
3	A	56	SER	N-CA-C	6.90	118.59	111.14
3	B	54	HIS	N-CA-C	-6.62	104.52	112.59
1	C	397	VAL	N-CA-C	6.44	117.19	110.62
2	F	49	PRO	CB-CA-C	-6.34	101.10	111.56
2	F	46	TYR	N-CA-C	6.00	123.59	110.80
1	D	112	ALA	CA-C-N	5.61	131.57	122.48
1	D	112	ALA	C-N-CA	5.61	131.57	122.48
1	C	395	ASP	N-CA-C	-5.58	104.89	110.97
3	B	54	HIS	N-CA-CB	5.39	119.55	110.92
2	F	15	CYS	CA-CB-SG	5.37	126.76	114.40
3	A	43	LEU	N-CA-C	5.03	116.72	108.52

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	83	1
1	D	2827	0	2875	115	1
2	E	340	0	327	37	1
2	F	340	0	327	62	0
3	A	3920	0	3971	129	1
3	B	3920	0	3972	137	2
All	All	14174	0	14347	492	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 (492) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:41:SER:OG	3:B:84:GLY:C	2.18	0.86
3:A:57:ASP:CG	1:D:217:ARG:NH2	2.34	0.86
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
1:D:85:HIS:CE1	2:F:47:HIS:HE1	1.95	0.81
3:A:57:ASP:CG	1:D:217:ARG:HH21	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:58:LEU:HD12	3:B:58:LEU:C	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:58:LEU:C	3:A:58:LEU:HD12	2.25	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: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
3:A:42:ASN:C	3:A:43:LEU:HD12	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:THR:OG1	1:D:116:CYS:SG	2.60	0.58
3:A:43:LEU:HD12	3:A:43:LEU:N	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
3:B:41:SER:HG	3:B:83:LEU:C	1.91	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
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
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:B:46:MET:HE2	3:B:81:LEU:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:A:46:MET:HE2	3:A:81:LEU:O	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:SER:HB2	3:A:103:GLN:HG2	1.92	0.51
1:D:304:ALA:HB1	1:D:306:MET:HE3	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:A:270:GLN:HE21	3:A:294:SER:HG	1.55	0.50
3:B:223:ARG:HG3	3:B:247:SER:O	2.11	0.50
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
3:B:330:LEU:HG	3:B:333:MET:HE3	1.93	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
1:D:88:GLU:CD	2:F:51:ARG:HB2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:304:ALA:HB1	1:C:306:MET:HE3	1.95	0.48
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:330:LEU:HG	3:A:333:MET:HE3	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
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
2:F:15:CYS:C	2:F:17:PRO:HD2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:46:MET:HE3	3:B:46:MET:HB3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:274:LEU:HD12	3:B:296:ASN:ND2	2.32	0.44
1:C:287:ARG:NH2	3:B:57:ASP:CG	2.75	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
3:B:50:TRP:CD1	3:B:50:TRP:H	2.36	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
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:88:GLU:CD	2:E:51:ARG:HB2	2.43	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:45:ASN:C	3:A:48:LEU:HG	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:LEU:HD22	3:A:333:MET:HE1	1.99	0.43
3:A:238:CYS:HB2	3:A:262:LEU:HD21	2.01	0.43
3:A:425:GLU:H	3:A:425:GLU:CD	2.26	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:58:LEU:C	3:B:58:LEU:CD1	2.91	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
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
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
3:B:425:GLU:H	3:B:425:GLU:CD	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:315:LEU:HD22	3:B:333:MET:HE1	2.01	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:111:THR:HG21	3:B:194:GLN:CD	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:304:ALA:HB1	1:D:306:MET:CE	2.51	0.40
3:B:345:LYS:HG2	3:B:369:ARG:NH1	2.36	0.40
1:C:177:GLU:CD	1:C:177:GLU:H	2.28	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%)	11	42
1	D	361/433 (83%)	317 (88%)	41 (11%)	3 (1%)	16	49
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%)	30	62
3	B	509/555 (92%)	437 (86%)	71 (14%)	1 (0%)	43	74
All	All	1822/2080 (88%)	1573 (86%)	231 (13%)	18 (1%)	12	44

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 ⓘ

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	320/378 (85%)	317 (99%)	3 (1%)	70	75
1	D	320/378 (85%)	317 (99%)	3 (1%)	70	75
2	E	39/45 (87%)	36 (92%)	3 (8%)	12	37
2	F	39/45 (87%)	35 (90%)	4 (10%)	7	28
3	A	450/485 (93%)	445 (99%)	5 (1%)	65	74
3	B	450/485 (93%)	438 (97%)	12 (3%)	39	62
All	All	1618/1816 (89%)	1588 (98%)	30 (2%)	50	67

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	296	LEU
1	C	394	ARG
1	C	396	THR
2	E	15	CYS
2	E	47	HIS
2	E	49	PRO
3	A	40	PHE
3	A	42	ASN
3	A	49	ASP
3	A	212	CYS
3	A	514	LEU
1	D	107	LEU
1	D	111	THR
1	D	296	LEU
3	B	40	PHE
3	B	41	SER
3	B	42	ASN
3	B	43	LEU
3	B	53	VAL
3	B	54	HIS
3	B	56	SER
3	B	58	LEU
3	B	211	MET
3	B	212	CYS
3	B	214	LEU
3	B	514	LEU
2	F	8	CYS

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Mol	Chain	Res	Type
2	F	15	CYS
2	F	47	HIS
2	F	49	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	GLN
1	C	147	GLN
1	C	168	ASN
1	C	180	ASN
3	A	54	HIS
3	A	154	GLN
3	A	263	GLN
3	A	364	ASN
3	A	367	ASN
3	A	412	ASN
3	A	502	GLN
3	A	511	ASN
3	A	530	ASN
3	A	536	ASN
1	D	58	GLN
1	D	85	HIS
1	D	180	ASN
3	B	77	ASN
3	B	263	GLN
3	B	364	ASN
3	B	367	ASN
3	B	412	ASN
3	B	502	GLN
3	B	511	ASN
3	B	530	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 [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(Å²)	Q<0.9
1	C	363/433 (83%)	0.39	14 (3%)	43	24	41, 56, 75, 85	0
1	D	363/433 (83%)	0.46	15 (4%)	41	23	40, 58, 74, 86	0
2	E	45/52 (86%)	0.61	2 (4%)	39	22	51, 72, 94, 99	0
2	F	45/52 (86%)	0.70	3 (6%)	24	15	51, 74, 96, 103	0
3	A	513/555 (92%)	0.23	11 (2%)	63	39	36, 49, 60, 76	0
3	B	513/555 (92%)	0.44	21 (4%)	41	23	40, 52, 83, 102	0
All	All	1842/2080 (88%)	0.39	66 (3%)	46	26	36, 53, 77, 103	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	142	LEU	4.6
1	C	343	PRO	4.4
3	B	75	SER	4.4
3	B	364	ASN	4.2
3	B	38	GLY	4.2
1	D	143	GLY	4.0
1	C	304	ALA	4.0
1	D	82	GLY	3.6
3	A	265	ALA	3.4
1	D	217	ARG	3.3
3	B	90	ALA	3.1
1	D	53	THR	3.1
3	B	43	LEU	3.0
1	C	355	LEU	2.9
1	C	367	PRO	2.9
1	D	128	THR	2.9
3	B	254	GLU	2.9
3	A	254	GLU	2.9
2	E	5	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	A	255	ILE	2.8
3	B	342	ASN	2.8
3	B	91	ILE	2.7
3	A	253	GLY	2.6
1	C	321	ALA	2.6
1	C	287	ARG	2.6
1	C	391	PRO	2.6
3	A	531	LEU	2.6
3	A	64	VAL	2.6
3	B	54	HIS	2.5
3	B	283	GLY	2.5
1	C	200	LEU	2.5
2	F	5	LEU	2.5
3	B	255	ILE	2.5
1	D	300	ASN	2.4
2	E	6	PRO	2.4
1	D	110	ASP	2.4
3	B	33	LEU	2.3
3	B	76	LEU	2.3
1	C	392	PHE	2.3
1	D	144	ARG	2.3
3	B	531	LEU	2.2
3	B	71	TYR	2.2
3	B	533	VAL	2.2
3	A	266	THR	2.2
2	F	4	SER	2.2
3	A	43	LEU	2.2
1	D	145	ALA	2.1
1	D	197	SER	2.1
1	D	402	ARG	2.1
3	B	478	ARG	2.1
1	C	264	VAL	2.1
3	A	504	LEU	2.1
3	B	119	ALA	2.1
1	D	271	SER	2.1
3	A	447	PRO	2.1
3	B	191	GLU	2.1
2	F	1	THR	2.1
1	D	83	ARG	2.1
1	C	306	MET	2.1
3	A	142	LEU	2.0
1	D	293	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	368	LEU	2.0
1	C	300	ASN	2.0
1	C	141	CYS	2.0
3	B	169	LEU	2.0
3	B	378	ILE	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.