



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 01:58 PM EDT

PDB ID : 3MP4
Title : Crystal structure of Human lyase R41M mutant
Authors : Fu, Z.; Runquist, J.A.; Montgomery, C.; Mizioro, H.M.; Kim, J.-J.P.
Deposited on : 2010-04-24
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

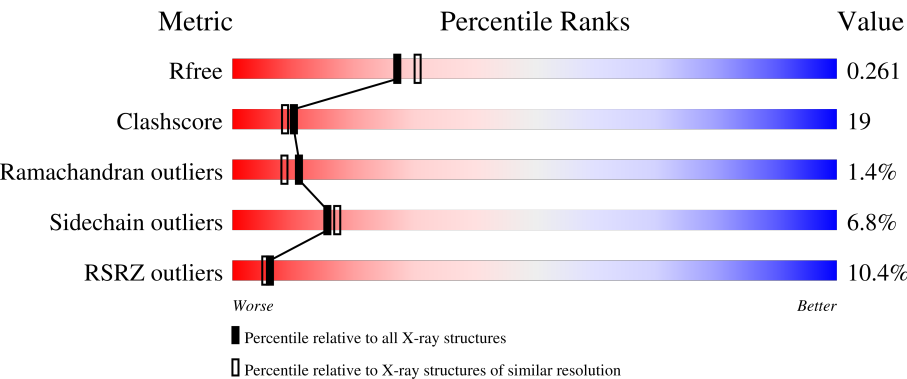
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	298	<div><div>3%</div><div>72%</div><div>23%</div><div>..</div></div>
1	B	298	<div><div>8%</div><div>70%</div><div>26%</div><div>..</div></div>
1	C	298	<div><div>15%</div><div>56%</div><div>39%</div><div>..</div></div>
1	D	298	<div><div>9%</div><div>68%</div><div>27%</div><div>..</div></div>
1	E	298	<div><div>5%</div><div>69%</div><div>26%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	298	<div><div></div><div>21%</div><div>55%</div><div>39%</div><div>• •</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13431 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 Hydroxymethylglutaryl-CoA lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2186	1389	362	417	18			
1	B	296	Total	C	N	O	S	0	0	0
			2186	1389	362	417	18			
1	C	296	Total	C	N	O	S	0	0	0
			2186	1389	362	417	18			
1	D	296	Total	C	N	O	S	0	0	0
			2186	1389	362	417	18			
1	E	296	Total	C	N	O	S	0	0	0
			2186	1389	362	417	18			
1	F	287	Total	C	N	O	S	0	0	0
			2119	1348	350	404	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	ARG	engineered mutation	UNP P35914
B	41	MET	ARG	engineered mutation	UNP P35914
C	41	MET	ARG	engineered mutation	UNP P35914
D	41	MET	ARG	engineered mutation	UNP P35914
E	41	MET	ARG	engineered mutation	UNP P35914
F	41	MET	ARG	engineered mutation	UNP P35914

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	98	Total	O	0	0
			98	98		
2	B	68	Total	O	0	0
			68	68		
2	C	34	Total	O	0	0
			34	34		

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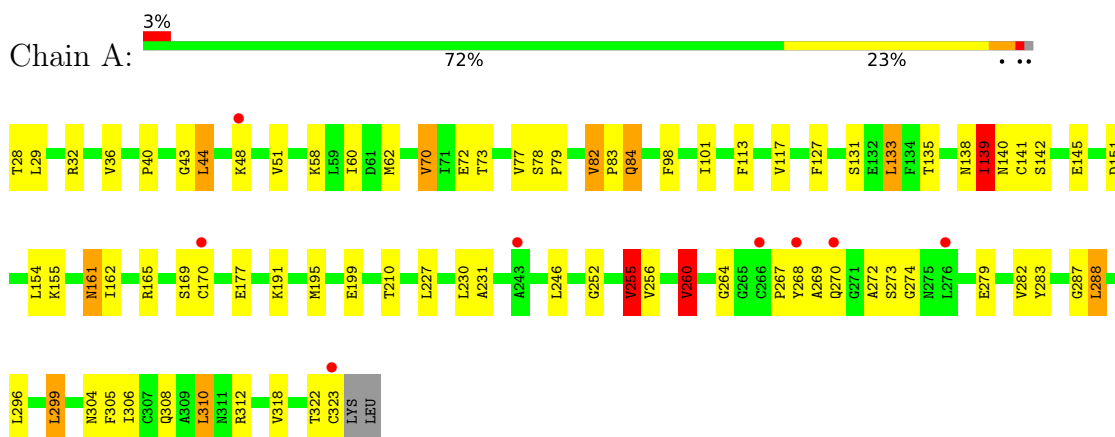
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	76	Total 76	O 76	0	0
2	E	78	Total 78	O 78	0	0
2	F	28	Total 28	O 28	0	0

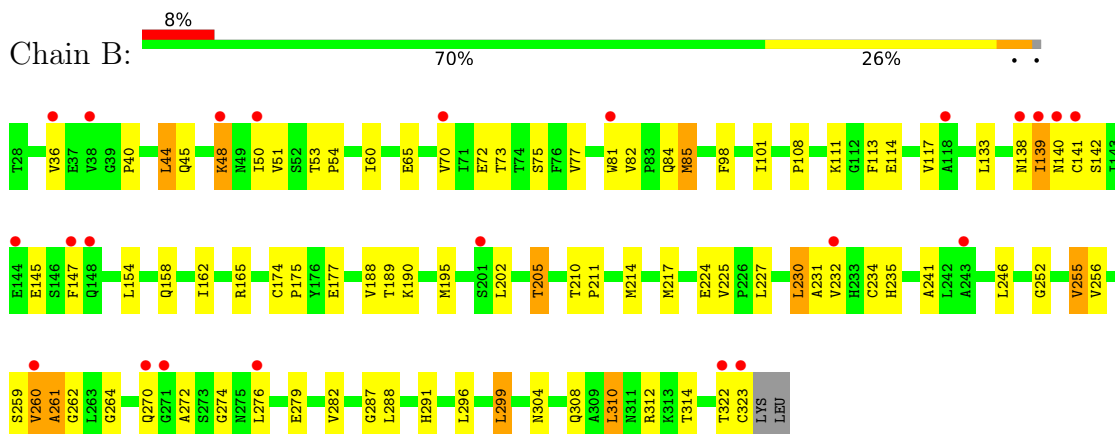
3 Residue-property plots [i](#)

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.

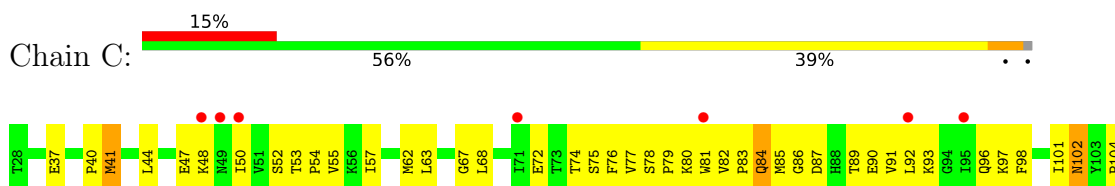
• Molecule 1: Hydroxymethylglutaryl-CoA lyase

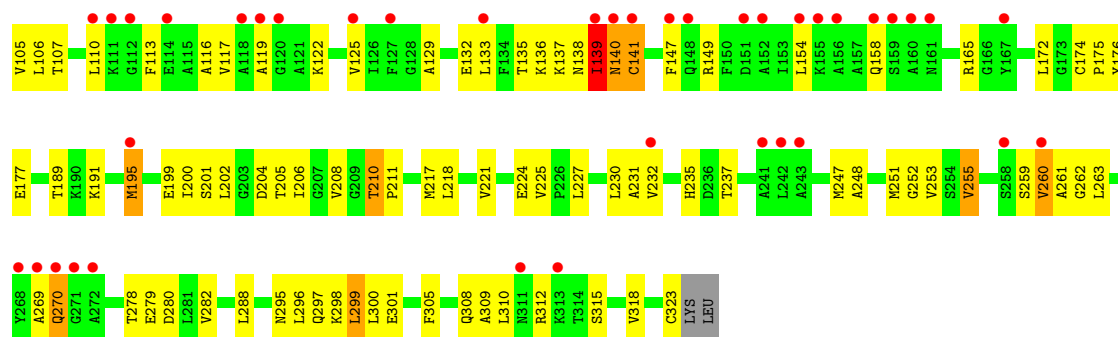


• Molecule 1: Hydroxymethylglutaryl-CoA lyase

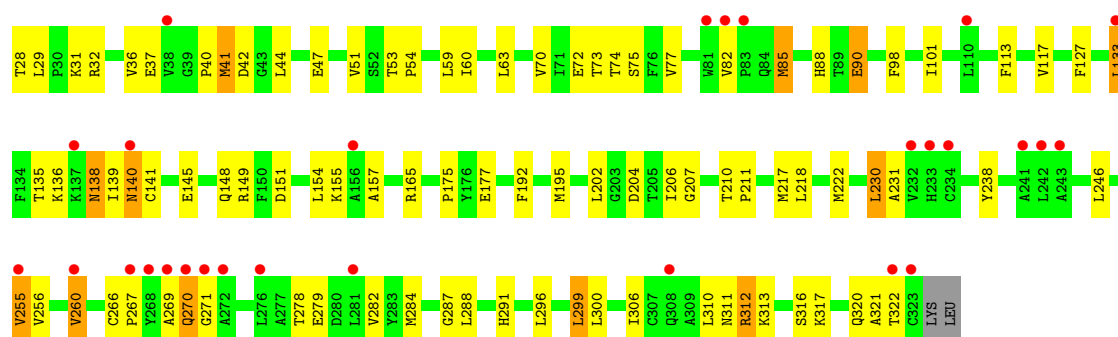


• Molecule 1: Hydroxymethylglutaryl-CoA lyase

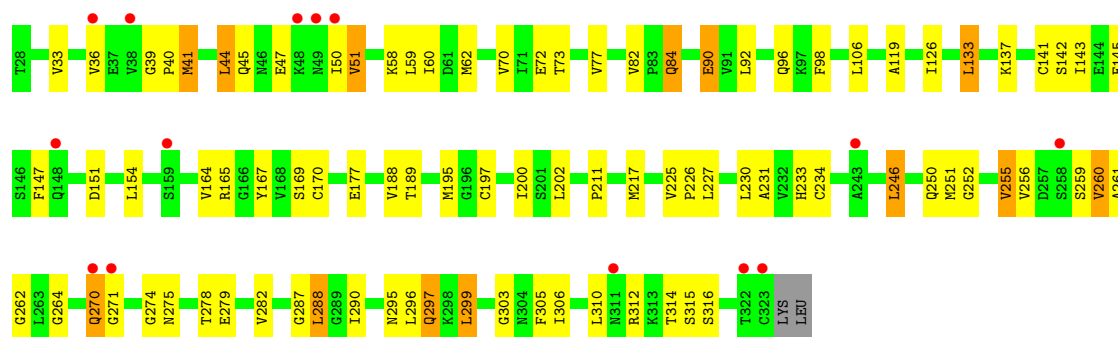




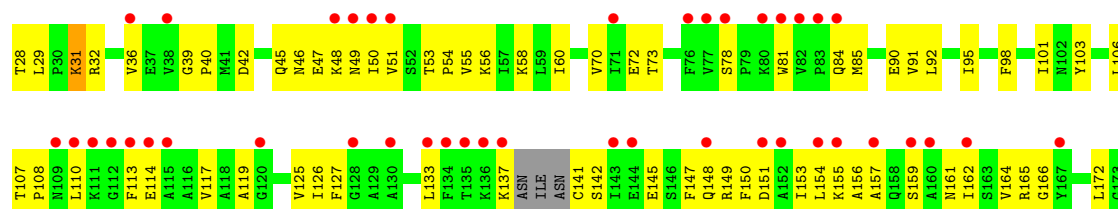
• Molecule 1: Hydroxymethylglutaryl-CoA lyase

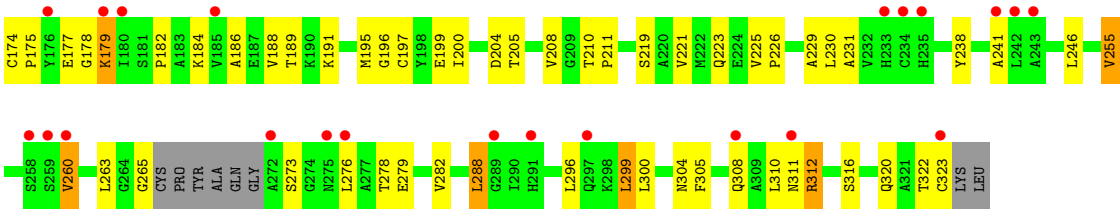


• Molecule 1: Hydroxymethylglutaryl-CoA lyase



• Molecule 1: Hydroxymethylglutaryl-CoA lyase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.49Å 116.62Å 86.98Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	29.16 – 2.20 29.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.16-2.20) 90.9 (29.16-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.261 0.219 , 0.261	Depositor DCC
R_{free} test set	8395 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	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	0.94	EDS
Total number of atoms	13431	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	A	0.41	0/2221	0.64	1/3007 (0.0%)
1	B	0.37	0/2221	0.60	0/3007
1	C	0.32	0/2221	0.56	0/3007
1	D	0.36	0/2221	0.59	0/3007
1	E	0.36	0/2221	0.59	0/3007
1	F	0.32	0/2150	0.55	0/2906
All	All	0.36	0/13255	0.59	1/17941 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	VAL	CA-CB-CG1	5.10	118.55	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2186	0	2240	77	0
1	B	2186	0	2240	63	0
1	C	2186	0	2240	123	0
1	D	2186	0	2240	75	0
1	E	2186	0	2240	75	0
1	F	2119	0	2178	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	98	0	0	1	0
2	B	68	0	0	4	0
2	C	34	0	0	2	0
2	D	76	0	0	3	0
2	E	78	0	0	2	0
2	F	28	0	0	1	0
All	All	13431	0	13378	500	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (500) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:VAL:HG13	1:C:82:VAL:HG11	1.29	1.10
1:A:28:THR:HG22	1:A:29:LEU:H	1.20	1.03
1:F:50:ILE:HG22	1:F:84:GLN:HG3	1.42	1.02
1:B:48:LYS:H	1:B:48:LYS:HD2	1.30	0.94
1:E:36:VAL:HA	1:E:70:VAL:HG13	1.51	0.92
1:F:31:LYS:H	1:F:31:LYS:HZ2	0.95	0.92
1:A:58:LYS:HG2	1:A:62:MET:HE2	1.54	0.90
1:D:36:VAL:HA	1:D:70:VAL:HG13	1.53	0.88
1:A:260:VAL:O	1:A:279:GLU:OE1	1.90	0.88
1:C:40:PRO:HA	1:C:44:LEU:HD23	1.57	0.86
1:C:211:PRO:HG2	1:D:288:LEU:HD21	1.58	0.85
1:E:58:LYS:HG2	1:E:62:MET:HE2	1.59	0.84
1:E:84:GLN:H	1:E:84:GLN:HE21	1.22	0.84
1:B:279:GLU:HG3	1:B:299:LEU:HD13	1.61	0.82
1:B:264:GLY:O	1:B:274:GLY:HA3	1.81	0.81
1:C:47:GLU:HG2	1:C:310:LEU:HD21	1.63	0.81
1:D:139:ILE:CG2	1:D:149:ARG:HH22	1.94	0.80
1:E:84:GLN:H	1:E:84:GLN:NE2	1.78	0.80
1:F:31:LYS:H	1:F:31:LYS:NZ	1.78	0.80
1:D:139:ILE:HG21	1:D:149:ARG:HH22	1.46	0.80
1:C:77:VAL:CG1	1:C:82:VAL:HG11	2.09	0.79
1:B:36:VAL:HG22	1:B:70:VAL:HG11	1.65	0.79
1:E:50:ILE:HG22	1:E:84:GLN:HG3	1.64	0.79
1:B:77:VAL:HB	1:B:108:PRO:HG3	1.63	0.78
1:D:36:VAL:HG22	1:D:70:VAL:HG11	1.66	0.78
1:A:279:GLU:HG3	1:A:299:LEU:HD13	1.66	0.78
1:E:36:VAL:HG22	1:E:70:VAL:HG11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PHE:O	1:C:117:VAL:HG23	1.84	0.77
1:C:78:SER:HB2	1:C:80:LYS:HG2	1.64	0.77
1:A:138:ASN:O	1:A:139:ILE:HG23	1.84	0.76
1:B:36:VAL:HA	1:B:70:VAL:HG13	1.67	0.76
1:C:102:ASN:N	1:C:102:ASN:HD22	1.81	0.76
1:A:141:CYS:HB2	1:A:145:GLU:HB2	1.66	0.76
1:D:231:ALA:HB2	1:D:255:VAL:HG22	1.68	0.76
1:B:282:VAL:HG21	1:B:296:LEU:HD13	1.67	0.75
1:A:58:LYS:HG2	1:A:62:MET:CE	2.17	0.74
1:E:154:LEU:HD13	1:E:195:MET:HB3	1.69	0.74
1:D:231:ALA:CB	1:D:255:VAL:HG22	2.16	0.74
1:F:78:SER:HB3	1:F:81:TRP:CD1	2.24	0.73
1:F:36:VAL:HA	1:F:70:VAL:HG13	1.71	0.72
1:C:40:PRO:HG2	1:C:72:GLU:O	1.90	0.72
1:D:154:LEU:HD13	1:D:195:MET:HB3	1.72	0.71
1:B:214:MET:CE	1:B:232:VAL:HG21	2.21	0.71
1:E:288:LEU:HD11	1:F:211:PRO:HD2	1.71	0.70
1:F:133:LEU:HB2	1:F:177:GLU:HG3	1.73	0.70
1:A:322:THR:O	1:A:323:CYS:HB2	1.89	0.70
1:F:31:LYS:HZ2	1:F:31:LYS:N	1.80	0.70
1:B:282:VAL:CG2	1:B:296:LEU:HD13	2.22	0.70
1:F:106:LEU:HD12	1:F:125:VAL:O	1.92	0.69
1:A:191:LYS:HE2	1:A:195:MET:CE	2.22	0.69
1:F:141:CYS:N	1:F:149:ARG:HH12	1.91	0.69
1:C:138:ASN:O	1:C:139:ILE:HG23	1.92	0.69
1:F:322:THR:O	1:F:323:CYS:HB2	1.92	0.69
1:B:75:SER:HB3	1:B:85:MET:HG2	1.73	0.69
1:A:28:THR:HG22	1:A:29:LEU:N	2.01	0.69
1:A:60:ILE:HD13	1:A:73:THR:HG23	1.74	0.69
1:E:282:VAL:HG21	1:E:296:LEU:HD13	1.74	0.69
1:F:60:ILE:HD13	1:F:73:THR:HG23	1.75	0.69
1:F:42:ASP:HA	1:F:45:GLN:HE21	1.58	0.69
1:C:279:GLU:HG3	1:C:299:LEU:HD13	1.75	0.68
1:D:151:ASP:O	1:D:155:LYS:HD3	1.93	0.68
1:C:87:ASP:O	1:C:91:VAL:HG23	1.92	0.68
1:E:40:PRO:HA	1:E:44:LEU:HD22	1.74	0.68
1:E:282:VAL:CG2	1:E:296:LEU:HD13	2.23	0.68
1:E:92:LEU:HD23	1:E:119:ALA:HB3	1.75	0.68
1:E:264:GLY:O	1:E:274:GLY:HA3	1.94	0.68
1:B:117:VAL:HG22	1:B:162:ILE:CD1	2.24	0.67
1:F:40:PRO:HG2	1:F:72:GLU:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:PHE:HB2	1:B:101:ILE:HD12	1.76	0.67
1:A:161:ASN:HD21	1:C:149:ARG:NH1	1.93	0.67
1:B:214:MET:HE3	1:B:232:VAL:HG21	1.77	0.66
1:B:142:SER:HB3	1:B:145:GLU:HG3	1.77	0.66
1:E:233:HIS:HE1	1:E:275:ASN:OD1	1.79	0.66
1:D:284:MET:O	1:D:288:LEU:HD23	1.94	0.66
1:D:40:PRO:HG2	1:D:72:GLU:O	1.95	0.66
1:D:47:GLU:HG2	1:D:310:LEU:HD21	1.77	0.66
1:D:41:MET:HE2	1:D:74:THR:HA	1.77	0.66
1:B:133:LEU:HD23	1:B:177:GLU:HG2	1.76	0.65
1:E:84:GLN:HE21	1:E:84:GLN:N	1.94	0.65
1:A:282:VAL:CG2	1:A:296:LEU:HD13	2.25	0.65
1:B:40:PRO:HG2	1:B:72:GLU:O	1.96	0.65
1:B:189:THR:HG22	1:B:225:VAL:HG21	1.78	0.65
1:E:260:VAL:O	1:E:279:GLU:OE1	2.15	0.65
1:B:60:ILE:HD13	1:B:73:THR:HG23	1.78	0.65
1:E:142:SER:OG	1:E:145:GLU:HG3	1.97	0.65
1:A:84:GLN:H	1:A:84:GLN:NE2	1.93	0.64
1:D:282:VAL:HG21	1:D:296:LEU:HD13	1.79	0.64
1:E:36:VAL:HA	1:E:70:VAL:CG1	2.27	0.64
1:A:40:PRO:HA	1:A:44:LEU:HD22	1.79	0.64
1:D:136:LYS:C	1:D:138:ASN:H	2.01	0.64
1:E:40:PRO:HG2	1:E:72:GLU:O	1.98	0.64
1:B:231:ALA:CB	1:B:255:VAL:HG22	2.28	0.63
1:F:137:LYS:HD2	1:F:137:LYS:N	2.13	0.63
1:A:191:LYS:HE2	1:A:195:MET:HE1	1.80	0.63
1:C:135:THR:HA	1:C:139:ILE:HD11	1.79	0.63
1:C:82:VAL:O	1:C:82:VAL:HG13	1.98	0.63
1:F:230:LEU:O	1:F:255:VAL:HG13	1.97	0.63
1:F:304:ASN:O	1:F:308:GLN:HG3	1.97	0.63
1:F:189:THR:HG22	1:F:225:VAL:HG21	1.79	0.63
1:A:282:VAL:HG21	1:A:296:LEU:HD13	1.80	0.63
1:B:154:LEU:HD13	1:B:195:MET:HB3	1.80	0.63
1:A:58:LYS:CG	1:A:62:MET:HE2	2.27	0.63
1:F:151:ASP:OD1	1:F:155:LYS:HD3	1.99	0.63
1:C:96:GLN:O	1:C:97:LYS:HD3	1.99	0.63
1:D:154:LEU:CD1	1:D:195:MET:HB3	2.28	0.63
1:F:47:GLU:HG2	1:F:310:LEU:HD21	1.81	0.63
1:A:77:VAL:HG11	1:A:82:VAL:HG11	1.81	0.62
1:F:186:ALA:HA	1:F:221:VAL:HG22	1.82	0.62
1:F:191:LYS:HG3	1:F:195:MET:HE1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PRO:HG2	1:A:84:GLN:HE21	1.64	0.61
1:C:138:ASN:C	1:C:139:ILE:HD13	2.20	0.61
1:F:154:LEU:HD13	1:F:195:MET:HB3	1.83	0.61
1:A:210:THR:HG21	1:B:287:GLY:HA3	1.82	0.61
1:C:154:LEU:O	1:C:158:GLN:HB2	2.01	0.61
1:B:291:HIS:HB2	2:B:763:HOH:O	2.00	0.61
1:F:172:LEU:HD12	1:F:204:ASP:HB2	1.82	0.61
1:B:50:ILE:HG22	1:B:84:GLN:HG3	1.82	0.60
1:E:279:GLU:OE1	1:E:279:GLU:N	2.34	0.60
1:F:36:VAL:HG22	1:F:70:VAL:HG11	1.83	0.60
1:C:53:THR:HG22	1:C:57:ILE:HD11	1.83	0.60
1:E:33:VAL:HG23	1:E:290:ILE:HG21	1.81	0.60
1:C:278:THR:O	1:C:282:VAL:HG13	2.02	0.60
1:C:279:GLU:HG2	1:C:300:LEU:HD23	1.83	0.60
1:F:282:VAL:CG2	1:F:296:LEU:HD13	2.31	0.60
1:B:259:SER:O	1:B:260:VAL:O	2.19	0.60
1:C:78:SER:HB2	1:C:80:LYS:CG	2.32	0.59
1:F:208:VAL:HG12	1:F:238:TYR:CE2	2.37	0.59
1:B:211:PRO:HD3	2:B:618:HOH:O	2.02	0.59
1:D:51:VAL:HG13	1:D:310:LEU:HD13	1.84	0.59
1:B:48:LYS:H	1:B:48:LYS:CD	2.04	0.59
1:B:40:PRO:HA	1:B:44:LEU:HD22	1.85	0.58
1:C:122:LYS:NZ	1:C:122:LYS:HB3	2.18	0.58
1:F:51:VAL:CG1	1:F:310:LEU:HD13	2.33	0.58
1:C:98:PHE:CB	1:C:101:ILE:HD12	2.33	0.58
1:C:154:LEU:HD13	1:C:195:MET:O	2.03	0.58
1:D:139:ILE:HG21	1:D:149:ARG:NH2	2.16	0.58
1:F:200:ILE:HD12	1:F:200:ILE:N	2.18	0.58
1:F:191:LYS:HG3	1:F:195:MET:CE	2.33	0.58
1:C:98:PHE:HB2	1:C:101:ILE:HD12	1.85	0.58
1:D:202:LEU:HD13	1:D:217:MET:SD	2.44	0.57
1:B:190:LYS:HD3	1:B:224:GLU:HB3	1.86	0.57
1:C:259:SER:OG	1:C:263:LEU:HB2	2.04	0.57
1:C:211:PRO:HD3	2:C:620:HOH:O	2.05	0.57
1:D:282:VAL:CG2	1:D:296:LEU:HD13	2.34	0.57
1:E:92:LEU:HD23	1:E:119:ALA:CB	2.34	0.57
1:E:51:VAL:HG13	1:E:310:LEU:HD12	1.87	0.57
1:C:129:ALA:HB3	1:C:135:THR:HG23	1.86	0.56
1:A:135:THR:HG22	1:A:141:CYS:O	2.04	0.56
1:C:282:VAL:CG2	1:C:296:LEU:HD13	2.36	0.56
1:E:231:ALA:CB	1:E:255:VAL:HG22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:LEU:HD22	1:E:306:ILE:HD13	1.86	0.56
1:A:28:THR:CG2	1:A:29:LEU:H	2.02	0.56
1:C:135:THR:O	1:C:139:ILE:HG12	2.05	0.56
1:A:306:ILE:HG13	1:A:310:LEU:CD2	2.36	0.56
1:C:37:GLU:OE2	1:C:260:VAL:HG23	2.04	0.56
1:A:62:MET:HE3	1:A:305:PHE:CD2	2.40	0.56
1:E:77:VAL:HG11	1:E:82:VAL:HG11	1.87	0.56
1:F:126:ILE:HD11	1:F:197:CYS:SG	2.46	0.56
1:D:211:PRO:HD3	2:D:671:HOH:O	2.06	0.56
1:A:231:ALA:CB	1:A:255:VAL:HG22	2.36	0.55
1:C:72:GLU:HA	1:C:104:PRO:HG2	1.88	0.55
1:C:53:THR:HG23	1:C:91:VAL:HG22	1.88	0.55
1:E:287:GLY:HA3	1:F:210:THR:HG21	1.89	0.55
1:A:40:PRO:HG2	1:A:72:GLU:O	2.07	0.55
1:C:53:THR:O	1:C:57:ILE:HG13	2.06	0.55
1:D:41:MET:HE3	1:D:75:SER:N	2.21	0.55
1:C:89:THR:HG22	1:C:93:LYS:HE2	1.89	0.55
1:C:231:ALA:CB	1:C:255:VAL:HG22	2.36	0.55
1:C:232:VAL:HG23	1:C:253:VAL:HG11	1.89	0.55
1:A:154:LEU:HD13	1:A:195:MET:HG2	1.87	0.55
1:C:82:VAL:HG22	1:C:85:MET:HB2	1.88	0.55
1:F:53:THR:N	1:F:54:PRO:HD2	2.22	0.55
1:C:78:SER:O	1:C:82:VAL:HG12	2.07	0.55
1:C:92:LEU:HD23	1:C:119:ALA:HB3	1.89	0.55
1:F:58:LYS:HD3	1:F:305:PHE:CZ	2.42	0.55
1:F:147:PHE:CE1	1:F:191:LYS:HG2	2.42	0.54
1:E:278:THR:HG22	1:E:299:LEU:HD11	1.89	0.54
1:A:279:GLU:HA	1:A:282:VAL:HG22	1.89	0.54
1:C:191:LYS:HE2	1:C:195:MET:CE	2.38	0.54
1:B:82:VAL:O	1:B:82:VAL:HG13	2.08	0.54
1:B:241:ALA:HB1	1:B:276:LEU:HB2	1.90	0.54
1:D:37:GLU:HG2	1:D:63:LEU:HD13	1.89	0.54
1:C:102:ASN:N	1:C:102:ASN:ND2	2.51	0.54
1:F:260:VAL:O	1:F:279:GLU:OE1	2.26	0.53
1:C:211:PRO:CG	1:D:288:LEU:HD21	2.35	0.53
1:C:262:GLY:HA3	1:C:315:SER:HB2	1.90	0.53
1:B:214:MET:HE1	1:B:232:VAL:HG21	1.90	0.53
1:C:76:PHE:CD2	1:C:116:ALA:HB2	2.43	0.53
1:F:113:PHE:HE2	1:F:157:ALA:HB2	1.73	0.53
1:B:322:THR:O	1:B:323:CYS:HB2	2.08	0.53
1:F:31:LYS:HZ3	1:F:31:LYS:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:CYS:SG	1:F:175:PRO:HD2	2.48	0.53
1:C:53:THR:N	1:C:54:PRO:HD2	2.23	0.52
1:C:83:PRO:HG2	1:C:84:GLN:NE2	2.24	0.52
1:C:41:MET:SD	1:C:41:MET:C	2.87	0.52
1:C:62:MET:HE3	1:C:305:PHE:CD2	2.44	0.52
1:C:74:THR:H	1:C:105:VAL:HG12	1.74	0.52
1:B:231:ALA:HB1	1:B:255:VAL:HG22	1.92	0.52
1:F:184:LYS:HE3	1:F:188:VAL:HG23	1.92	0.52
1:A:141:CYS:HA	1:A:145:GLU:OE2	2.08	0.52
1:F:133:LEU:HD13	1:F:137:LYS:NZ	2.24	0.52
1:F:145:GLU:O	1:F:148:GLN:HB2	2.10	0.52
1:F:51:VAL:HG13	1:F:310:LEU:HD13	1.91	0.52
1:A:58:LYS:HE3	1:A:305:PHE:CE1	2.45	0.52
1:C:154:LEU:CD1	1:C:195:MET:HG2	2.39	0.52
1:E:47:GLU:HG2	1:E:310:LEU:HD21	1.90	0.52
1:F:39:GLY:N	1:F:40:PRO:HD2	2.25	0.52
1:B:113:PHE:CZ	1:B:162:ILE:HD12	2.45	0.52
1:B:133:LEU:HD23	1:B:177:GLU:CG	2.40	0.52
1:D:279:GLU:HG2	1:D:300:LEU:HD23	1.92	0.52
1:C:191:LYS:O	1:C:195:MET:HB2	2.10	0.52
1:E:189:THR:HG22	1:E:225:VAL:HG21	1.92	0.52
1:E:279:GLU:O	1:E:282:VAL:HG22	2.10	0.52
1:E:126:ILE:HD11	1:E:197:CYS:SG	2.50	0.51
1:E:227:LEU:HD21	1:E:252:GLY:HA3	1.91	0.51
1:E:96:GLN:HB2	1:E:98:PHE:HE1	1.76	0.51
1:F:166:GLY:O	1:F:200:ILE:HA	2.11	0.51
1:D:139:ILE:O	1:D:140:ASN:HB2	2.11	0.51
1:C:37:GLU:HB2	1:C:68:LEU:CD1	2.41	0.51
1:C:280:ASP:OD1	1:C:318:VAL:HG23	2.11	0.51
1:B:48:LYS:HD2	1:B:48:LYS:N	2.13	0.51
1:C:133:LEU:HD13	1:C:177:GLU:OE1	2.11	0.51
1:A:191:LYS:O	1:A:195:MET:HB2	2.10	0.51
1:F:46:ASN:HB3	1:F:265:GLY:H	1.75	0.51
1:E:141:CYS:HB2	1:E:145:GLU:OE1	2.11	0.50
1:F:322:THR:O	1:F:323:CYS:CB	2.58	0.50
1:A:84:GLN:H	1:A:84:GLN:CD	2.15	0.50
1:C:63:LEU:HD21	1:C:260:VAL:HG22	1.93	0.50
1:C:308:GLN:C	1:C:310:LEU:H	2.15	0.50
1:C:132:GLU:HB3	1:C:136:LYS:NZ	2.27	0.50
1:C:210:THR:HG21	1:D:287:GLY:HA3	1.92	0.50
1:F:42:ASP:HA	1:F:45:GLN:NE2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD21	1:A:252:GLY:HA3	1.92	0.50
1:C:204:ASP:HA	2:C:629:HOH:O	2.12	0.50
1:D:135:THR:HG22	1:D:141:CYS:O	2.11	0.50
1:F:164:VAL:O	1:F:197:CYS:HA	2.11	0.50
1:B:53:THR:N	1:B:54:PRO:HD2	2.27	0.50
1:B:231:ALA:HB2	1:B:255:VAL:HG22	1.94	0.50
1:C:52:SER:OG	1:C:55:VAL:HG23	2.11	0.50
1:E:231:ALA:HB2	1:E:255:VAL:HG22	1.93	0.50
1:E:270:GLN:CD	1:E:270:GLN:H	2.13	0.50
1:F:98:PHE:HB2	1:F:101:ILE:HD12	1.93	0.50
1:B:85:MET:HA	1:B:85:MET:HE2	1.93	0.50
1:B:154:LEU:O	1:B:158:GLN:HG3	2.11	0.50
1:C:295:ASN:OD1	1:C:298:LYS:HG3	2.12	0.49
1:F:229:ALA:C	1:F:230:LEU:HD12	2.33	0.49
1:D:136:LYS:C	1:D:138:ASN:N	2.65	0.49
1:F:145:GLU:C	1:F:149:ARG:HH11	2.15	0.49
1:A:154:LEU:CD1	1:A:195:MET:HG2	2.42	0.49
1:E:133:LEU:HB2	1:E:177:GLU:HG3	1.93	0.49
1:A:62:MET:HE1	1:A:305:PHE:CG	2.48	0.49
1:A:77:VAL:HG11	1:A:82:VAL:CG1	2.41	0.49
1:A:304:ASN:O	1:A:308:GLN:HG3	2.12	0.49
1:A:113:PHE:O	1:A:117:VAL:HG23	2.13	0.49
1:B:260:VAL:O	1:B:262:GLY:N	2.37	0.49
1:C:230:LEU:O	1:C:255:VAL:HG13	2.13	0.49
1:D:88:HIS:HE1	2:D:724:HOH:O	1.96	0.49
1:A:264:GLY:O	1:A:274:GLY:HA3	2.12	0.49
1:D:60:ILE:HD13	1:D:73:THR:HG23	1.95	0.49
1:E:47:GLU:HG2	1:E:310:LEU:CD2	2.42	0.49
1:C:101:ILE:C	1:C:102:ASN:HD22	2.16	0.49
1:C:251:MET:HA	1:C:251:MET:CE	2.42	0.49
1:F:241:ALA:HB1	1:F:276:LEU:HB2	1.95	0.49
1:A:58:LYS:HE3	1:A:62:MET:HE1	1.93	0.49
1:B:205:THR:O	1:B:235:HIS:ND1	2.34	0.49
1:D:133:LEU:HD23	1:D:177:GLU:HG2	1.95	0.49
1:E:58:LYS:HG2	1:E:62:MET:CE	2.39	0.49
1:E:96:GLN:HB2	1:E:98:PHE:CE1	2.48	0.49
1:F:51:VAL:HG23	1:F:56:LYS:HG3	1.94	0.49
1:C:137:LYS:HD2	1:C:176:TYR:CZ	2.48	0.48
1:F:31:LYS:NZ	1:F:31:LYS:HB2	2.27	0.48
1:F:137:LYS:HD2	1:F:137:LYS:H	1.75	0.48
1:D:51:VAL:CG1	1:D:310:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:ARG:HD2	1:F:199:GLU:OE2	2.12	0.48
1:C:139:ILE:HD13	1:C:139:ILE:N	2.27	0.48
1:C:279:GLU:HG2	1:C:300:LEU:CD2	2.43	0.48
1:A:282:VAL:HG23	1:A:296:LEU:HD13	1.95	0.48
1:F:58:LYS:HD3	1:F:305:PHE:CE1	2.48	0.48
1:C:147:PHE:CE1	1:C:191:LYS:HG2	2.47	0.48
1:D:32:ARG:HB3	1:D:291:HIS:HB3	1.95	0.48
1:C:217:MET:O	1:C:221:VAL:HG23	2.13	0.48
1:D:279:GLU:O	1:D:282:VAL:HG22	2.13	0.48
1:E:143:ILE:O	1:E:147:PHE:HD1	1.97	0.48
1:A:142:SER:OG	1:A:145:GLU:HG3	2.13	0.48
1:A:161:ASN:HD21	1:C:149:ARG:CZ	2.26	0.48
1:E:62:MET:HE3	1:E:305:PHE:CD2	2.49	0.48
1:F:92:LEU:HD23	1:F:119:ALA:CB	2.43	0.48
1:C:282:VAL:HG21	1:C:296:LEU:HD13	1.96	0.48
1:D:155:LYS:HD2	1:D:155:LYS:N	2.29	0.48
1:E:39:GLY:N	1:E:40:PRO:HD2	2.29	0.48
1:F:91:VAL:O	1:F:95:ILE:HG23	2.13	0.48
1:C:106:LEU:O	1:C:107:THR:HG23	2.13	0.47
1:C:139:ILE:C	1:C:141:CYS:H	2.17	0.47
1:F:127:PHE:N	1:F:127:PHE:CD1	2.80	0.47
1:A:273:SER:HB2	2:A:555:HOH:O	2.14	0.47
1:C:189:THR:HG22	1:C:225:VAL:HG21	1.96	0.47
1:D:90:GLU:H	1:D:90:GLU:CD	2.18	0.47
1:E:303:GLY:O	1:E:306:ILE:HG22	2.13	0.47
1:F:28:THR:HG23	1:F:29:LEU:N	2.28	0.47
1:A:169:SER:O	1:A:170:CYS:SG	2.71	0.47
1:A:48:LYS:H	1:A:48:LYS:HD2	1.78	0.47
1:D:36:VAL:HA	1:D:70:VAL:CG1	2.36	0.47
1:E:51:VAL:HG13	1:E:310:LEU:CD1	2.44	0.47
1:C:75:SER:HA	1:C:106:LEU:HB2	1.95	0.47
1:D:41:MET:HE1	1:D:85:MET:SD	2.54	0.47
1:D:218:LEU:O	1:D:222:MET:HG3	2.15	0.47
1:F:154:LEU:CD1	1:F:195:MET:HB3	2.43	0.47
1:C:84:GLN:CD	1:C:84:GLN:H	2.17	0.47
1:C:132:GLU:HB3	1:C:136:LYS:HZ3	1.80	0.47
1:C:202:LEU:HD13	1:C:217:MET:SD	2.55	0.47
1:C:297:GLN:O	1:C:301:GLU:HG3	2.15	0.47
1:D:260:VAL:O	1:D:279:GLU:OE1	2.33	0.47
1:F:156:ALA:O	1:F:159:SER:HB2	2.14	0.47
1:A:77:VAL:CG1	1:A:82:VAL:CG1	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ILE:CD1	1:D:73:THR:HG23	2.44	0.47
1:C:84:GLN:NE2	1:C:84:GLN:H	2.13	0.47
1:D:316:SER:O	1:D:320:GLN:HG3	2.14	0.47
1:A:117:VAL:HG22	1:A:162:ILE:CD1	2.45	0.47
1:B:272:ALA:HB1	2:B:871:HOH:O	2.14	0.47
1:C:41:MET:HG3	1:C:106:LEU:HD13	1.97	0.47
1:D:175:PRO:HB3	1:D:206:ILE:HG21	1.96	0.47
1:C:191:LYS:HE2	1:C:195:MET:HE1	1.97	0.46
1:F:231:ALA:CB	1:F:255:VAL:HG22	2.45	0.46
1:C:79:PRO:HG3	1:C:86:GLY:HA2	1.97	0.46
1:C:227:LEU:HD21	1:C:252:GLY:HA3	1.96	0.46
1:E:90:GLU:HG3	2:E:714:HOH:O	2.16	0.46
1:A:138:ASN:C	1:A:139:ILE:HG12	2.35	0.46
1:C:247:MET:HE3	1:C:247:MET:O	2.14	0.46
1:E:39:GLY:HA2	1:E:259:SER:OG	2.15	0.46
1:E:200:ILE:N	1:E:200:ILE:HD12	2.31	0.46
1:F:73:THR:OG1	1:F:103:TYR:HB3	2.16	0.46
1:F:191:LYS:O	1:F:195:MET:HG3	2.16	0.46
1:F:199:GLU:C	1:F:200:ILE:HD12	2.35	0.46
1:D:77:VAL:HG11	1:D:82:VAL:HG11	1.97	0.46
1:F:50:ILE:CG2	1:F:84:GLN:HG3	2.30	0.46
1:F:90:GLU:OE1	1:F:90:GLU:N	2.47	0.46
1:A:270:GLN:OE1	1:B:323:CYS:HA	2.16	0.46
1:E:167:TYR:CE1	1:E:233:HIS:HD2	2.34	0.46
1:E:295:ASN:OD1	1:E:297:GLN:HG2	2.14	0.46
1:A:165:ARG:HD2	1:A:199:GLU:OE2	2.16	0.46
1:D:269:ALA:O	1:D:270:GLN:C	2.53	0.46
1:C:237:THR:HG22	1:D:321:ALA:HB2	1.96	0.46
1:F:182:PRO:HD2	2:F:776:HOH:O	2.16	0.46
1:D:207:GLY:O	1:D:238:TYR:HD2	1.99	0.46
1:E:41:MET:O	1:E:45:GLN:HB2	2.16	0.46
1:D:51:VAL:HG13	1:D:310:LEU:CD1	2.45	0.46
1:F:178:GLY:O	1:F:179:LYS:C	2.54	0.46
1:C:90:GLU:HA	1:C:93:LYS:HE2	1.98	0.46
1:D:47:GLU:HG2	1:D:310:LEU:CD2	2.43	0.46
1:D:270:GLN:HB2	1:D:271:GLY:H	1.52	0.46
1:E:142:SER:HG	1:E:145:GLU:HG3	1.81	0.46
1:F:92:LEU:HD23	1:F:119:ALA:HB3	1.98	0.46
1:F:110:LEU:O	1:F:113:PHE:HB3	2.16	0.46
1:B:304:ASN:O	1:B:308:GLN:HG3	2.16	0.45
1:C:92:LEU:HD23	1:C:119:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:MET:HE1	1:E:45:GLN:OE1	2.15	0.45
1:A:82:VAL:HG22	1:A:82:VAL:O	2.16	0.45
1:F:279:GLU:O	1:F:282:VAL:HG22	2.15	0.45
1:A:231:ALA:HB2	1:A:255:VAL:HG22	1.97	0.45
1:B:147:PHE:HZ	1:B:188:VAL:HG13	1.81	0.45
1:C:172:LEU:HD12	1:C:204:ASP:HB2	1.98	0.45
1:D:260:VAL:HG13	1:D:299:LEU:CD2	2.45	0.45
1:E:261:ALA:HB1	1:E:314:THR:OG1	2.17	0.45
1:F:219:SER:O	1:F:223:GLN:HG2	2.17	0.45
1:F:282:VAL:HG21	1:F:296:LEU:HD13	1.97	0.45
1:C:122:LYS:HB3	1:C:122:LYS:HZ2	1.81	0.45
1:D:210:THR:HB	1:D:211:PRO:HD2	1.97	0.45
1:C:78:SER:C	1:C:80:LYS:H	2.19	0.45
1:D:266:CYS:HA	1:D:267:PRO:HD3	1.84	0.45
1:F:117:VAL:HG22	1:F:162:ILE:CD1	2.47	0.45
1:B:227:LEU:HD21	1:B:252:GLY:HA3	1.99	0.45
1:C:218:LEU:CD1	1:C:248:ALA:HA	2.47	0.45
1:B:202:LEU:HD13	1:B:217:MET:SD	2.57	0.45
1:B:261:ALA:HB1	1:B:314:THR:OG1	2.16	0.45
1:C:37:GLU:HG2	1:C:63:LEU:HD13	1.99	0.45
1:C:53:THR:HG22	1:C:57:ILE:CD1	2.47	0.45
1:B:98:PHE:CB	1:B:101:ILE:HD12	2.46	0.45
1:C:136:LYS:HA	1:C:140:ASN:HA	1.98	0.45
1:C:200:ILE:N	1:C:200:ILE:HD12	2.32	0.45
1:E:278:THR:O	1:E:282:VAL:HG13	2.17	0.45
1:F:113:PHE:O	1:F:117:VAL:HG23	2.17	0.44
1:F:151:ASP:HA	1:F:154:LEU:HD12	1.98	0.44
1:A:62:MET:CE	1:A:305:PHE:CD2	3.00	0.44
1:D:317:LYS:HD3	1:D:320:GLN:OE1	2.17	0.44
1:B:165:ARG:HD3	2:B:877:HOH:O	2.17	0.44
1:C:133:LEU:HA	1:C:136:LYS:HB2	2.00	0.44
1:D:28:THR:OG1	1:D:29:LEU:N	2.47	0.44
1:D:312:ARG:HD3	1:D:313:LYS:O	2.17	0.44
1:A:139:ILE:HD12	1:A:141:CYS:SG	2.58	0.44
1:C:110:LEU:O	1:C:113:PHE:HB3	2.17	0.44
1:C:154:LEU:HD13	1:C:195:MET:HG2	1.99	0.44
1:F:230:LEU:HD12	1:F:230:LEU:N	2.32	0.44
1:F:278:THR:HG22	1:F:299:LEU:HD11	1.99	0.44
1:A:51:VAL:HG13	1:A:310:LEU:HD13	1.99	0.44
1:E:90:GLU:OE1	1:E:90:GLU:N	2.51	0.44
1:C:82:VAL:CG2	1:C:85:MET:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:N	1:C:133:LEU:HD12	2.33	0.44
1:E:154:LEU:HD23	1:E:164:VAL:HG21	1.98	0.43
1:F:226:PRO:O	1:F:230:LEU:HD13	2.18	0.43
1:C:67:GLY:O	1:C:68:LEU:C	2.55	0.43
1:D:41:MET:HG3	1:D:72:GLU:HG2	2.00	0.43
1:E:154:LEU:CD1	1:E:195:MET:HB3	2.41	0.43
1:E:246:LEU:HD22	1:E:250:GLN:HG3	2.00	0.43
1:A:98:PHE:HB2	1:A:101:ILE:HD12	1.99	0.43
1:C:41:MET:CB	1:C:72:GLU:HG2	2.48	0.43
1:C:78:SER:C	1:C:80:LYS:N	2.71	0.43
1:A:77:VAL:HG13	1:A:82:VAL:HG13	2.00	0.43
1:C:206:ILE:HG13	1:C:208:VAL:HG13	1.99	0.43
1:D:145:GLU:HA	1:D:148:GLN:OE1	2.17	0.43
1:A:267:PRO:C	1:A:269:ALA:H	2.20	0.43
1:C:125:VAL:HG22	1:C:165:ARG:HB3	2.01	0.43
1:F:184:LYS:HE3	1:F:188:VAL:CG2	2.48	0.43
1:F:279:GLU:HG2	1:F:300:LEU:HD23	2.00	0.43
1:C:107:THR:CG2	1:C:113:PHE:HA	2.48	0.43
1:D:113:PHE:HZ	1:D:157:ALA:HA	1.84	0.43
1:F:263:LEU:HD23	1:F:312:ARG:CZ	2.49	0.43
1:D:98:PHE:HB2	1:D:101:ILE:HD12	2.00	0.43
1:D:140:ASN:HD22	1:D:140:ASN:HA	1.57	0.43
1:E:270:GLN:CD	1:E:270:GLN:N	2.71	0.43
1:F:51:VAL:HB	1:F:55:VAL:HG11	2.01	0.43
1:A:142:SER:H	1:A:145:GLU:CD	2.22	0.43
1:C:37:GLU:HB2	1:C:68:LEU:HD11	2.01	0.43
1:C:199:GLU:C	1:C:200:ILE:HD12	2.39	0.43
1:D:36:VAL:HG22	1:D:70:VAL:CG1	2.44	0.43
1:D:133:LEU:HB2	1:D:177:GLU:HG3	2.01	0.43
1:F:142:SER:HB3	1:F:145:GLU:CG	2.48	0.43
1:C:269:ALA:O	1:C:270:GLN:C	2.57	0.42
1:D:231:ALA:HB1	1:D:255:VAL:HG22	1.97	0.42
1:E:211:PRO:HG2	1:F:288:LEU:CD1	2.49	0.42
1:F:157:ALA:HB1	1:F:162:ILE:O	2.19	0.42
1:E:60:ILE:HD13	1:E:73:THR:HG23	2.01	0.42
1:E:41:MET:O	1:E:41:MET:HE2	2.19	0.42
1:A:306:ILE:HG13	1:A:310:LEU:HD23	2.02	0.42
1:B:45:GLN:HG3	1:B:82:VAL:HG21	2.01	0.42
1:B:174:CYS:SG	1:B:175:PRO:HD2	2.60	0.42
1:B:232:VAL:HG22	1:B:234:CYS:SG	2.59	0.42
1:C:40:PRO:HA	1:C:44:LEU:CD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:SER:HA	1:C:231:ALA:HB3	2.01	0.42
1:A:43:GLY:HA2	1:A:264:GLY:HA3	2.02	0.42
1:C:90:GLU:HA	1:C:93:LYS:CE	2.50	0.42
1:C:205:THR:O	1:C:235:HIS:ND1	2.49	0.42
1:D:278:THR:HG22	1:D:299:LEU:HD11	2.00	0.42
1:F:133:LEU:HD13	1:F:137:LYS:HZ3	1.84	0.42
1:A:288:LEU:HD11	1:B:211:PRO:HB2	2.02	0.42
1:B:139:ILE:O	1:B:141:CYS:N	2.51	0.42
1:D:279:GLU:HG2	1:D:300:LEU:CD2	2.49	0.42
1:F:47:GLU:HG2	1:F:310:LEU:CD2	2.47	0.42
1:B:260:VAL:C	1:B:262:GLY:H	2.20	0.41
1:E:188:VAL:HG23	1:E:189:THR:N	2.35	0.41
1:E:226:PRO:O	1:E:230:LEU:CD2	2.68	0.41
1:F:46:ASN:CB	1:F:265:GLY:H	2.33	0.41
1:B:111:LYS:O	1:B:114:GLU:HB3	2.18	0.41
1:C:50:ILE:HD12	1:C:84:GLN:HA	2.02	0.41
1:E:202:LEU:HD13	1:E:217:MET:SD	2.61	0.41
1:A:127:PHE:CD1	1:A:127:PHE:N	2.88	0.41
1:A:139:ILE:O	1:A:141:CYS:N	2.53	0.41
1:C:37:GLU:OE2	1:C:260:VAL:N	2.48	0.41
1:D:59:LEU:HD13	1:D:306:ILE:HB	2.02	0.41
1:D:279:GLU:HG3	1:D:299:LEU:HD13	2.02	0.41
1:E:41:MET:HG3	1:E:106:LEU:HD13	2.03	0.41
1:E:106:LEU:N	1:E:106:LEU:HD12	2.35	0.41
1:A:78:SER:HA	1:A:79:PRO:HD3	1.94	0.41
1:A:135:THR:HG23	1:A:139:ILE:HD11	2.02	0.41
1:E:59:LEU:HD22	1:E:306:ILE:CD1	2.50	0.41
1:A:83:PRO:HG2	1:A:84:GLN:NE2	2.32	0.41
1:A:131:SER:HB3	1:A:170:CYS:SG	2.60	0.41
1:A:133:LEU:HB2	1:A:177:GLU:HG3	2.02	0.41
1:D:230:LEU:O	1:D:255:VAL:HG13	2.20	0.41
1:F:148:GLN:C	1:F:150:PHE:H	2.23	0.41
1:C:139:ILE:HB	1:C:149:ARG:HH22	1.85	0.41
1:D:204:ASP:HA	2:D:615:HOH:O	2.20	0.41
1:E:279:GLU:HB2	1:E:316:SER:OG	2.20	0.41
1:F:107:THR:HA	1:F:108:PRO:HD2	1.95	0.41
1:F:151:ASP:O	1:F:155:LYS:HB2	2.20	0.41
1:A:36:VAL:HG13	1:A:70:VAL:CG2	2.51	0.41
1:A:270:GLN:C	1:A:272:ALA:H	2.24	0.41
1:D:41:MET:HB3	1:D:42:ASP:H	1.72	0.41
1:A:287:GLY:HA3	1:B:210:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ALA:O	1:C:315:SER:HB2	2.20	0.41
1:D:53:THR:N	1:D:54:PRO:HD2	2.35	0.41
1:D:139:ILE:O	1:D:139:ILE:HG22	2.21	0.41
1:F:113:PHE:CD2	1:F:153:ILE:HG23	2.55	0.41
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.96	0.41
1:C:93:LYS:HB2	1:C:93:LYS:HE3	1.90	0.40
1:C:139:ILE:HB	1:C:149:ARG:NH2	2.36	0.40
1:E:234:CYS:HB3	2:E:546:HOH:O	2.20	0.40
1:A:161:ASN:HD22	1:A:161:ASN:HA	1.54	0.40
1:B:139:ILE:C	1:B:141:CYS:H	2.23	0.40
1:E:169:SER:O	1:E:170:CYS:HB2	2.21	0.40
1:F:133:LEU:HD23	1:F:177:GLU:HG2	2.03	0.40
1:A:151:ASP:O	1:A:155:LYS:HD3	2.22	0.40
1:C:174:CYS:SG	1:C:175:PRO:HD2	2.62	0.40
1:D:113:PHE:O	1:D:117:VAL:HG23	2.21	0.40
1:E:133:LEU:O	1:E:137:LYS:HB2	2.21	0.40
1:F:316:SER:O	1:F:320:GLN:HG3	2.21	0.40
1:B:117:VAL:HG22	1:B:162:ILE:HD11	2.02	0.40
1:B:230:LEU:O	1:B:255:VAL:HG13	2.21	0.40
1:E:262:GLY:HA3	1:E:315:SER:HB2	2.03	0.40
1:A:283:TYR:HB2	1:A:318:VAL:HG21	2.04	0.40
1:F:288:LEU:HD12	1:F:288:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/298 (99%)	281 (96%)	10 (3%)	3 (1%)	15 14
1	B	294/298 (99%)	281 (96%)	8 (3%)	5 (2%)	9 6
1	C	294/298 (99%)	271 (92%)	18 (6%)	5 (2%)	9 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	294/298 (99%)	280 (95%)	11 (4%)	3 (1%)	15	14
1	E	294/298 (99%)	282 (96%)	9 (3%)	3 (1%)	15	14
1	F	281/298 (94%)	258 (92%)	18 (6%)	5 (2%)	8	5
All	All	1751/1788 (98%)	1653 (94%)	74 (4%)	24 (1%)	11	8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	260	VAL
1	B	260	VAL
1	C	270	GLN
1	D	260	VAL
1	D	270	GLN
1	E	260	VAL
1	F	260	VAL
1	B	261	ALA
1	B	270	GLN
1	C	139	ILE
1	C	260	VAL
1	E	271	GLY
1	F	48	LYS
1	F	273	SER
1	A	140	ASN
1	B	140	ASN
1	C	309	ALA
1	E	270	GLN
1	F	179	LYS
1	C	48	LYS
1	D	322	THR
1	B	139	ILE
1	F	196	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/240 (99%)	220 (92%)	18 (8%)	13	14
1	B	238/240 (99%)	222 (93%)	16 (7%)	16	18
1	C	238/240 (99%)	223 (94%)	15 (6%)	18	20
1	D	238/240 (99%)	220 (92%)	18 (8%)	13	14
1	E	238/240 (99%)	222 (93%)	16 (7%)	16	18
1	F	231/240 (96%)	218 (94%)	13 (6%)	21	25
All	All	1421/1440 (99%)	1325 (93%)	96 (7%)	16	17

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	44	LEU
1	A	70	VAL
1	A	82	VAL
1	A	84	GLN
1	A	133	LEU
1	A	139	ILE
1	A	161	ASN
1	A	230	LEU
1	A	246	LEU
1	A	255	VAL
1	A	256	VAL
1	A	260	VAL
1	A	268	TYR
1	A	288	LEU
1	A	299	LEU
1	A	310	LEU
1	A	312	ARG
1	B	44	LEU
1	B	48	LYS
1	B	51	VAL
1	B	65	GLU
1	B	81	TRP
1	B	85	MET
1	B	138	ASN
1	B	205	THR
1	B	230	LEU
1	B	246	LEU
1	B	255	VAL
1	B	256	VAL

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Mol	Chain	Res	Type
1	B	288	LEU
1	B	299	LEU
1	B	310	LEU
1	B	312	ARG
1	C	41	MET
1	C	81	TRP
1	C	84	GLN
1	C	102	ASN
1	C	139	ILE
1	C	140	ASN
1	C	141	CYS
1	C	195	MET
1	C	210	THR
1	C	224	GLU
1	C	255	VAL
1	C	288	LEU
1	C	299	LEU
1	C	312	ARG
1	C	323	CYS
1	D	31	LYS
1	D	41	MET
1	D	44	LEU
1	D	85	MET
1	D	90	GLU
1	D	127	PHE
1	D	133	LEU
1	D	138	ASN
1	D	140	ASN
1	D	165	ARG
1	D	192	PHE
1	D	230	LEU
1	D	246	LEU
1	D	255	VAL
1	D	256	VAL
1	D	299	LEU
1	D	311	ASN
1	D	312	ARG
1	E	41	MET
1	E	44	LEU
1	E	51	VAL
1	E	84	GLN
1	E	90	GLU

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Mol	Chain	Res	Type
1	E	133	LEU
1	E	151	ASP
1	E	165	ARG
1	E	246	LEU
1	E	251	MET
1	E	255	VAL
1	E	256	VAL
1	E	288	LEU
1	E	297	GLN
1	E	299	LEU
1	E	312	ARG
1	F	31	LYS
1	F	32	ARG
1	F	49	ASN
1	F	85	MET
1	F	114	GLU
1	F	161	ASN
1	F	205	THR
1	F	246	LEU
1	F	255	VAL
1	F	288	LEU
1	F	299	LEU
1	F	311	ASN
1	F	312	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	88	HIS
1	A	140	ASN
1	A	161	ASN
1	A	223	GLN
1	A	235	HIS
1	A	244	ASN
1	A	250	GLN
1	A	291	HIS
1	A	311	ASN
1	B	138	ASN
1	B	161	ASN
1	B	223	GLN
1	B	244	ASN

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	297	GLN
1	B	311	ASN
1	C	84	GLN
1	C	102	ASN
1	C	223	GLN
1	C	244	ASN
1	C	250	GLN
1	C	297	GLN
1	C	311	ASN
1	D	102	ASN
1	D	138	ASN
1	D	140	ASN
1	D	161	ASN
1	D	244	ASN
1	D	250	GLN
1	D	297	GLN
1	D	311	ASN
1	E	84	GLN
1	E	102	ASN
1	E	140	ASN
1	E	223	GLN
1	E	233	HIS
1	E	244	ASN
1	E	250	GLN
1	E	291	HIS
1	E	297	GLN
1	E	304	ASN
1	E	311	ASN
1	F	45	GLN
1	F	46	ASN
1	F	161	ASN
1	F	223	GLN
1	F	233	HIS
1	F	244	ASN
1	F	250	GLN
1	F	291	HIS
1	F	297	GLN
1	F	311	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/298 (99%)	0.07	8 (2%) 54 52	20, 32, 54, 69	0
1	B	296/298 (99%)	0.43	23 (7%) 13 11	25, 40, 70, 84	0
1	C	296/298 (99%)	0.87	46 (15%) 2 1	31, 57, 76, 80	0
1	D	296/298 (99%)	0.34	28 (9%) 8 7	25, 38, 68, 79	0
1	E	296/298 (99%)	0.23	14 (4%) 31 30	26, 40, 62, 78	0
1	F	287/298 (96%)	1.08	64 (22%) 0 0	36, 58, 82, 88	0
All	All	1767/1788 (98%)	0.50	183 (10%) 6 5	20, 42, 74, 88	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	ILE	6.9
1	F	81	TRP	6.8
1	E	270	GLN	6.7
1	F	137	LYS	5.7
1	F	176	TYR	5.6
1	F	159	SER	5.5
1	F	110	LEU	5.2
1	C	152	ALA	5.2
1	C	118	ALA	5.2
1	C	50	ILE	5.0
1	F	114	GLU	4.9
1	F	134	PHE	4.7
1	C	160	ALA	4.7
1	C	48	LYS	4.7
1	F	157	ALA	4.5
1	C	147	PHE	4.3
1	B	50	ILE	4.3
1	B	140	ASN	4.2
1	F	38	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	48	LYS	4.2
1	C	270	GLN	4.2
1	F	160	ALA	4.2
1	C	161	ASN	4.2
1	F	80	LYS	4.1
1	B	138	ASN	4.0
1	F	272	ALA	3.9
1	F	133	LEU	3.9
1	B	323	CYS	3.9
1	D	83	PRO	3.8
1	B	141	CYS	3.8
1	D	270	GLN	3.8
1	B	147	PHE	3.7
1	F	51	VAL	3.7
1	A	270	GLN	3.7
1	F	136	LYS	3.7
1	C	155	LYS	3.7
1	E	323	CYS	3.6
1	A	268	TYR	3.6
1	D	323	CYS	3.6
1	C	271	GLY	3.6
1	F	82	VAL	3.6
1	B	81	TRP	3.6
1	B	271	GLY	3.6
1	F	48	LYS	3.6
1	E	322	THR	3.6
1	D	137	LYS	3.5
1	F	143	ILE	3.5
1	D	81	TRP	3.5
1	C	140	ASN	3.5
1	F	113	PHE	3.5
1	D	241	ALA	3.5
1	C	167	TYR	3.5
1	B	139	ILE	3.4
1	C	243	ALA	3.4
1	F	180	ILE	3.4
1	F	77	VAL	3.3
1	E	48	LYS	3.2
1	C	268	TYR	3.2
1	C	119	ALA	3.2
1	C	311	ASN	3.2
1	E	159	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	81	TRP	3.2
1	D	140	ASN	3.2
1	B	36	VAL	3.2
1	D	243	ALA	3.2
1	F	233	HIS	3.1
1	F	49	ASN	3.0
1	F	258	SER	3.0
1	C	111	LYS	3.0
1	D	242	LEU	3.0
1	F	109	ASN	3.0
1	F	84	GLN	3.0
1	B	243	ALA	2.9
1	F	243	ALA	2.9
1	D	271	GLY	2.9
1	F	308	GLN	2.9
1	F	259	SER	2.9
1	C	120	GLY	2.9
1	B	270	GLN	2.9
1	E	50	ILE	2.8
1	C	110	LEU	2.8
1	C	269	ALA	2.8
1	E	243	ALA	2.8
1	F	276	LEU	2.8
1	C	195	MET	2.8
1	C	112	GLY	2.8
1	C	92	LEU	2.7
1	E	311	ASN	2.7
1	F	323	CYS	2.7
1	C	141	CYS	2.7
1	B	260	VAL	2.7
1	E	36	VAL	2.7
1	F	111	LYS	2.7
1	F	151	ASP	2.7
1	C	158	GLN	2.7
1	F	152	ALA	2.7
1	A	323	CYS	2.7
1	D	281	LEU	2.7
1	F	289	GLY	2.7
1	F	76	PHE	2.7
1	A	243	ALA	2.6
1	C	272	ALA	2.6
1	A	170	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	233	HIS	2.6
1	D	269	ALA	2.6
1	B	232	VAL	2.6
1	C	127	PHE	2.6
1	F	275	ASN	2.6
1	B	276	LEU	2.5
1	D	38	VAL	2.5
1	D	268	TYR	2.5
1	F	179	LYS	2.5
1	F	162	ILE	2.5
1	B	38	VAL	2.5
1	F	120	GLY	2.5
1	F	260	VAL	2.5
1	F	83	PRO	2.5
1	F	148	GLN	2.5
1	F	234	CYS	2.5
1	D	276	LEU	2.5
1	D	110	LEU	2.5
1	D	260	VAL	2.4
1	B	148	GLN	2.4
1	D	322	THR	2.4
1	F	128	GLY	2.4
1	C	95	ILE	2.4
1	C	148	GLN	2.4
1	C	156	ALA	2.4
1	F	241	ALA	2.4
1	C	114	GLU	2.4
1	C	71	ILE	2.4
1	D	133	LEU	2.4
1	F	112	GLY	2.4
1	F	291	HIS	2.4
1	E	148	GLN	2.4
1	D	267	PRO	2.4
1	F	135	THR	2.4
1	D	82	VAL	2.4
1	A	266	CYS	2.4
1	E	258	SER	2.4
1	F	130	ALA	2.3
1	C	154	LEU	2.3
1	D	234	CYS	2.3
1	C	49	ASN	2.3
1	F	155	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	271	GLY	2.3
1	C	232	VAL	2.3
1	C	260	VAL	2.3
1	F	154	LEU	2.3
1	B	70	VAL	2.3
1	A	48	LYS	2.2
1	B	118	ALA	2.2
1	A	276	LEU	2.2
1	C	258	SER	2.2
1	F	36	VAL	2.2
1	D	308	GLN	2.2
1	F	235	HIS	2.1
1	F	71	ILE	2.1
1	C	313	LYS	2.1
1	F	311	ASN	2.1
1	D	255	VAL	2.1
1	F	242	LEU	2.1
1	B	144	GLU	2.1
1	F	144	GLU	2.1
1	D	232	VAL	2.1
1	F	167	TYR	2.1
1	F	185	VAL	2.1
1	C	139	ILE	2.1
1	D	272	ALA	2.1
1	F	115	ALA	2.1
1	E	49	ASN	2.0
1	C	241	ALA	2.0
1	D	156	ALA	2.0
1	B	201	SER	2.0
1	C	159	SER	2.0
1	E	38	VAL	2.0
1	F	297	GLN	2.0
1	C	151	ASP	2.0
1	B	322	THR	2.0
1	F	78	SER	2.0
1	C	125	VAL	2.0
1	C	133	LEU	2.0
1	C	242	LEU	2.0

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

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.