



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:40 AM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

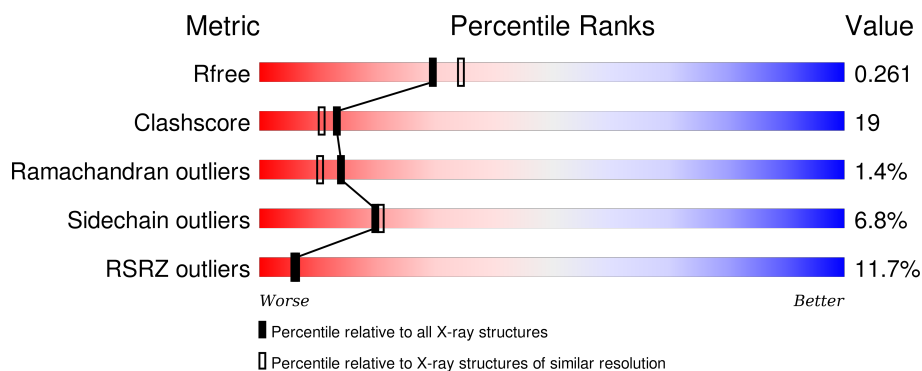
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>4%</div> <div>72%</div> <div>23%</div> <div>...</div> </div>
1	B	298	<div> <div>9%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	C	298	<div> <div>18%</div> <div>56%</div> <div>39%</div> <div>..</div> </div>
1	D	298	<div> <div>10%</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>24%</div><div>55%</div><div>39%</div><div></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	UNP P35914
B	41	MET	ARG	ENGINEERED	UNP P35914
C	41	MET	ARG	ENGINEERED	UNP P35914
D	41	MET	ARG	ENGINEERED	UNP P35914
E	41	MET	ARG	ENGINEERED	UNP P35914
F	41	MET	ARG	ENGINEERED	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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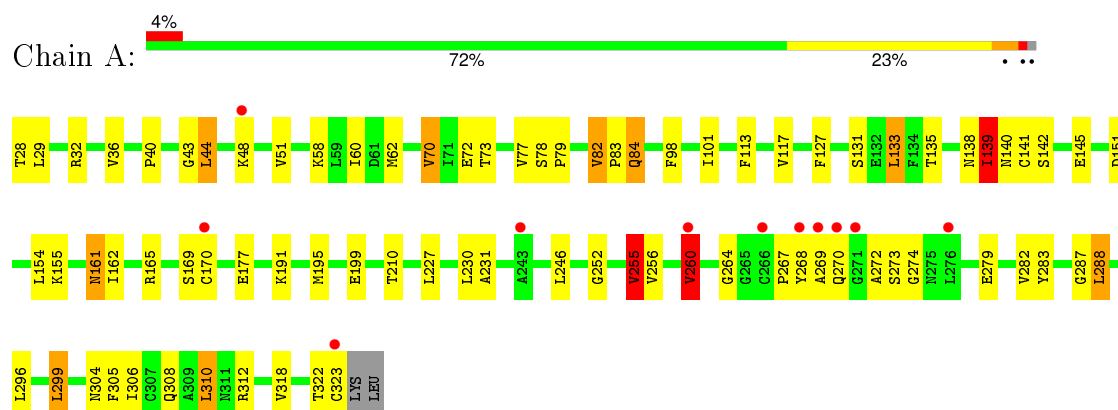
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	76	Total 76	O 76	0	0
2	E	78	Total 78	O 78	0	0
2	F	28	Total 28	O 28	0	0

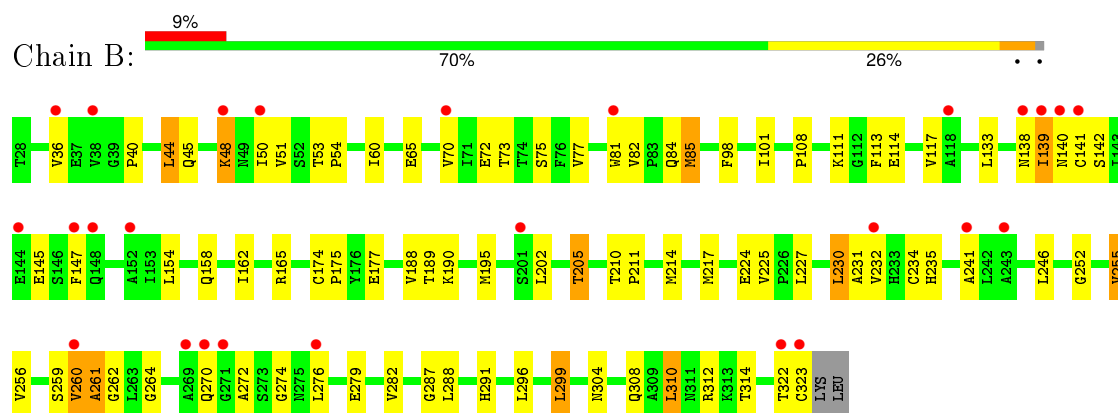
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

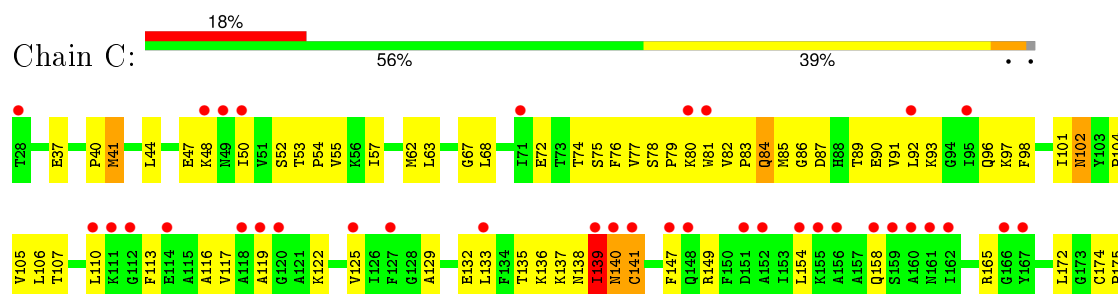
• Molecule 1: Hydroxymethylglutaryl-CoA lyase

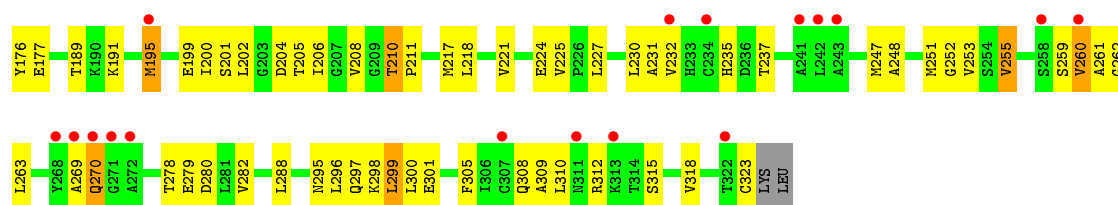


• Molecule 1: Hydroxymethylglutaryl-CoA lyase

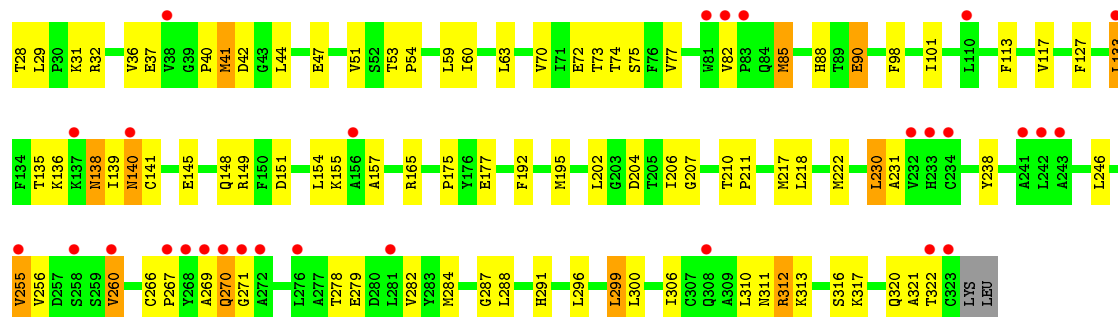


• Molecule 1: Hydroxymethylglutaryl-CoA lyase

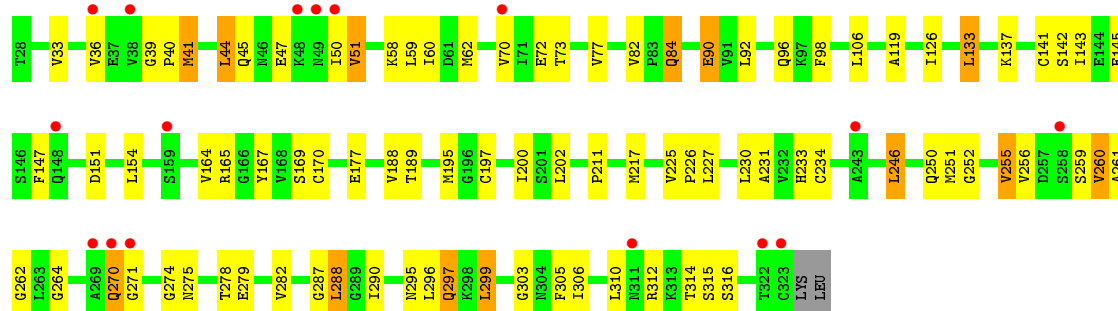




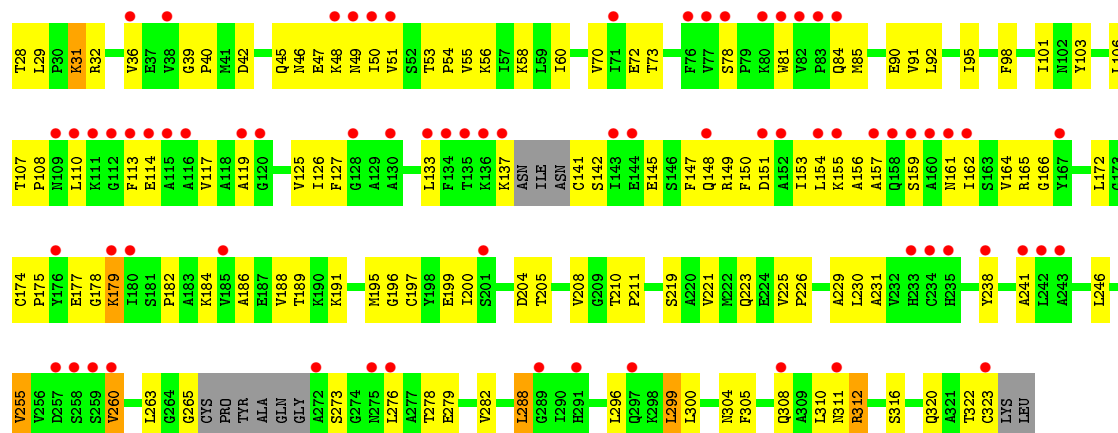
• Molecule 1: Hydroxymethylglutaryl-CoA lyase



• 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	196.49 Å 116.62 Å 86.98 Å 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 2.20 Å)	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 (10.05%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 83683 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:HD2	1:B:48:LYS:H	1.30	0.94
1:F:31:LYS:HZ2	1:F:31:LYS:H	0.95	0.92
1:E:36:VAL:HA	1:E:70:VAL:HG13	1.51	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:HE21	1:E:84:GLN:H	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:E:84:GLN:NE2	1:E:84:GLN:H	1.78	0.80
1:D:139:ILE:CG2	1:D:149:ARG:HH22	1.94	0.80
1:F:31:LYS:NZ	1:F:31:LYS:H	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:E:36:VAL:HG22	1:E:70:VAL:HG11	1.66	0.78
1:A:279:GLU:HG3	1:A:299:LEU:HD13	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:B:36:VAL:HA	1:B:70:VAL:HG13	1.67	0.76
1:A:138:ASN:O	1:A:139:ILE:HG23	1.84	0.76
1:C:102:ASN:HD22	1:C:102:ASN:N	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:F:31:LYS:HZ2	1:F:31:LYS:N	1.80	0.70
1:A:322:THR:O	1:A:323:CYS:HB2	1.89	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:F:141:CYS:N	1:F:149:ARG:HH12	1.91	0.69
1:A:191:LYS:HE2	1:A:195:MET:CE	2.22	0.69
1:F:322:THR:O	1:F:323:CYS:HB2	1.92	0.69
1:C:138:ASN:O	1:C:139:ILE:HG23	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:F:60:ILE:HD13	1:F:73:THR:HG23	1.75	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: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:282:VAL:CG2	1:E:296:LEU:HD13	2.23	0.68
1:E:40:PRO:HA	1:E:44:LEU:HD22	1.74	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:E:84:GLN:HE21	1:E:84:GLN:N	1.94	0.65
1:B:133:LEU:HD23	1:B:177:GLU:HG2	1.76	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:E:142:SER:OG	1:E:145:GLU:HG3	1.97	0.65
1:B:60:ILE:HD13	1:B:73:THR:HG23	1.78	0.65
1:A:84:GLN:NE2	1:A:84:GLN:H	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:F:137:LYS:HD2	1:F:137:LYS:N	2.13	0.63
1:B:231:ALA:CB	1:B:255:VAL:HG22	2.28	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:D:154:LEU:CD1	1:D:195:MET:HB3	2.28	0.63
1:C:96:GLN:O	1:C:97:LYS:HD3	1.99	0.63
1:F:47:GLU:HG2	1:F:310:LEU:HD21	1.81	0.63
1:F:186:ALA:HA	1:F:221:VAL:HG22	1.82	0.62
1:A:77:VAL:HG11	1:A:82:VAL:HG11	1.81	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:F:172:LEU:HD12	1:F:204:ASP:HB2	1.82	0.61
1:B:291:HIS:HB2	2:B:763:HOH:O	2.00	0.61
1:E:279:GLU:OE1	1:E:279:GLU:N	2.34	0.60
1:B:50:ILE:HG22	1:B:84:GLN:HG3	1.82	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:D:51:VAL:HG13	1:D:310:LEU:HD13	1.84	0.59
1:B:211:PRO:HD3	2:B:618:HOH:O	2.02	0.59
1:B:48:LYS:CD	1:B:48:LYS:H	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:N	1:F:200:ILE:HD12	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:C:259:SER:OG	1:C:263:LEU:HB2	2.04	0.57
1:B:190:LYS:HD3	1:B:224:GLU:HB3	1.86	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:C:37:GLU:OE2	1:C:260:VAL:HG23	2.04	0.56
1:A:306:ILE:HG13	1:A:310:LEU:CD2	2.36	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:C:72:GLU:HA	1:C:104:PRO:HG2	1.88	0.55
1:A:231:ALA:CB	1:A:255:VAL:HG22	2.36	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: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:A:40:PRO:HG2	1:A:72:GLU:O	2.07	0.55
1:C:89:THR:HG22	1:C:93:LYS:HE2	1.89	0.55
1:C:232:VAL:HG23	1:C:253:VAL:HG11	1.89	0.55
1:C:231:ALA:CB	1:C:255:VAL:HG22	2.36	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:241:ALA:HB1	1:B:276:LEU:HB2	1.90	0.54
1:B:82:VAL:HG13	1:B:82:VAL:O	2.08	0.54
1:D:37:GLU:HG2	1:D:63:LEU:HD13	1.89	0.54
1:C:102:ASN:ND2	1:C:102:ASN:N	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:F:113:PHE:HE2	1:F:157:ALA:HB2	1.73	0.53
1:C:76:PHE:CD2	1:C:116:ALA:HB2	2.43	0.53
1:F:31:LYS:HB2	1:F:31:LYS:HZ3	1.73	0.53
1:B:322:THR:O	1:B:323:CYS:HB2	2.08	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:C	1:C:41:MET:SD	2.87	0.52
1:C:74:THR:H	1:C:105:VAL:HG12	1.74	0.52
1:C:62:MET:HE3	1:C:305:PHE:CD2	2.44	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:F:39:GLY:N	1:F:40:PRO:HD2	2.25	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: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:E:279:GLU:O	1:E:282:VAL:HG22	2.10	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: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:F:322:THR:O	1:F:323:CYS:CB	2.58	0.50
1:E:141:CYS:HB2	1:E:145:GLU:OE1	2.11	0.50
1:C:308:GLN:C	1:C:310:LEU:H	2.15	0.50
1:A:84:GLN:CD	1:A:84:GLN:H	2.15	0.50
1:C:63:LEU:HD21	1:C:260:VAL:HG22	1.93	0.50
1:C:132:GLU:HB3	1:C:136:LYS:NZ	2.27	0.50
1:F:42:ASP:HA	1:F:45:GLN:NE2	2.24	0.50
1:C:210:THR:HG21	1:D:287:GLY:HA3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:VAL:O	1:F:197:CYS:HA	2.11	0.50
1:D:135:THR:HG22	1:D:141:CYS:O	2.11	0.50
1:C:204:ASP:HA	2:C:629:HOH:O	2.12	0.50
1:A:227:LEU:HD21	1:A:252:GLY:HA3	1.92	0.50
1:B:231:ALA:HB2	1:B:255:VAL:HG22	1.94	0.50
1:E:231:ALA:HB2	1:E:255:VAL:HG22	1.93	0.50
1:F:98:PHE:HB2	1:F:101:ILE:HD12	1.93	0.50
1:B:53:THR:N	1:B:54:PRO:HD2	2.27	0.50
1:E:270:GLN:H	1:E:270:GLN:CD	2.13	0.50
1:C:52:SER:OG	1:C:55:VAL:HG23	2.11	0.50
1:B:85:MET:HE2	1:B:85:MET:HA	1.93	0.50
1:B:154:LEU:O	1:B:158:GLN:HG3	2.11	0.50
1:F:229:ALA:C	1:F:230:LEU:HD12	2.33	0.49
1:C:295:ASN:OD1	1:C:298:LYS:HG3	2.12	0.49
1:F:145:GLU:C	1:F:149:ARG:HH11	2.15	0.49
1:D:136:LYS:C	1:D:138:ASN:N	2.65	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:E:47:GLU:HG2	1:E:310:LEU:CD2	2.42	0.49
1:D:60:ILE:HD13	1:D:73:THR:HG23	1.95	0.49
1:A:264:GLY:O	1:A:274:GLY:HA3	2.12	0.49
1:C:101:ILE:C	1:C:102:ASN:HD22	2.16	0.49
1:C:251:MET:CE	1:C:251:MET:HA	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:E:58:LYS:HG2	1:E:62:MET:CE	2.39	0.49
1:F:51:VAL:HG23	1:F:56:LYS:HG3	1.94	0.49
1:E:96:GLN:HB2	1:E:98:PHE:CE1	2.48	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:F:31:LYS:HB2	1:F:31:LYS:NZ	2.27	0.48
1:F:137:LYS:HD2	1:F:137:LYS:H	1.75	0.48
1:C:137:LYS:HD2	1:C:176:TYR:CZ	2.48	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:N	1:C:139:ILE:HD13	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: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:C:217:MET:O	1:C:221:VAL:HG23	2.13	0.48
1:E:62:MET:HE3	1:E:305:PHE:CD2	2.49	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:F:92:LEU:HD23	1:F:119:ALA:CB	2.43	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:C:282:VAL:HG21	1:C:296:LEU:HD13	1.96	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:E:303:GLY:O	1:E:306:ILE:HG22	2.13	0.47
1:C:189:THR:HG22	1:C:225:VAL:HG21	1.96	0.47
1:A:273:SER:HB2	2:A:555:HOH:O	2.14	0.47
1:D:90:GLU:H	1:D:90:GLU:CD	2.18	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: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:A:48:LYS:HD2	1:A:48:LYS:H	1.78	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:F:154:LEU:CD1	1:F:195:MET:HB3	2.43	0.47
1:D:218:LEU:O	1:D:222:MET:HG3	2.15	0.47
1:D:260:VAL:O	1:D:279:GLU:OE1	2.33	0.47
1:C:84:GLN:H	1:C:84:GLN:CD	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:F:156:ALA:O	1:F:159:SER:HB2	2.14	0.47
1:C:297:GLN:O	1:C:301:GLU:HG3	2.15	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:H	1:C:84:GLN:NE2	2.13	0.47
1:D:316:SER:O	1:D:320:GLN:HG3	2.14	0.47
1:C:41:MET:HG3	1:C:106:LEU:HD13	1.97	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:D:175:PRO:HB3	1:D:206:ILE:HG21	1.96	0.47
1:F:231:ALA:CB	1:F:255:VAL:HG22	2.45	0.46
1:C:191:LYS:HE2	1:C:195:MET:HE1	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:C:79:PRO:HG3	1:C:86:GLY:HA2	1.97	0.46
1:A:138:ASN:C	1:A:139:ILE:HG12	2.35	0.46
1:F:73:THR:OG1	1:F:103:TYR:HB3	2.16	0.46
1:E:39:GLY:HA2	1:E:259:SER:OG	2.15	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:E:200:ILE:HD12	1:E:200:ILE:N	2.31	0.46
1:C:247:MET:HE3	1:C:247:MET:O	2.14	0.46
1:F:50:ILE:CG2	1:F:84:GLN:HG3	2.30	0.46
1:D:77:VAL:HG11	1:D:82:VAL:HG11	1.97	0.46
1:F:90:GLU:OE1	1:F:90:GLU:N	2.47	0.46
1:E:167:TYR:CE1	1:E:233:HIS:HD2	2.34	0.46
1:A:270:GLN:OE1	1:B:323:CYS:HA	2.16	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:D:47:GLU:HG2	1:D:310:LEU:CD2	2.43	0.46
1:E:142:SER:HG	1:E:145:GLU:HG3	1.81	0.46
1:C:90:GLU:HA	1:C:93:LYS:HE2	1.98	0.46
1:F:110:LEU:O	1:F:113:PHE:HB3	2.16	0.46
1:F:92:LEU:HD23	1:F:119:ALA:HB3	1.98	0.46
1:D:270:GLN:HB2	1:D:271:GLY:H	1.52	0.46
1:C:92:LEU:HD23	1:C:119:ALA:CB	2.46	0.45
1:E:41:MET:HE1	1:E:45:GLN:OE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASN:O	1:B:308:GLN:HG3	2.16	0.45
1:A:82:VAL:O	1:A:82:VAL:HG22	2.16	0.45
1:F:279:GLU:O	1:F:282:VAL:HG22	2.15	0.45
1:D:260:VAL:HG13	1:D:299:LEU:CD2	2.45	0.45
1:A:231:ALA:HB2	1:A:255:VAL:HG22	1.97	0.45
1:C:172:LEU:HD12	1:C:204:ASP:HB2	1.98	0.45
1:E:261:ALA:HB1	1:E:314:THR:OG1	2.17	0.45
1:B:147:PHE:HZ	1:B:188:VAL:HG13	1.81	0.45
1:F:282:VAL:HG21	1:F:296:LEU:HD13	1.97	0.45
1:F:219:SER:O	1:F:223:GLN:HG2	2.17	0.45
1:C:122:LYS:HZ2	1:C:122:LYS:HB3	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:F:117:VAL:HG22	1:F:162:ILE:CD1	2.47	0.45
1:D:266:CYS:HA	1:D:267:PRO:HD3	1.84	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:C:53:THR:HG22	1:C:57:ILE:CD1	2.47	0.45
1:C:37:GLU:HG2	1:C:63:LEU:HD13	1.99	0.45
1:B:261:ALA:HB1	1:B:314:THR:OG1	2.16	0.45
1:B:202:LEU:HD13	1:B:217:MET:SD	2.57	0.45
1:E:278:THR:O	1:E:282:VAL:HG13	2.17	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:HD12	1:C:200:ILE:N	2.32	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:C:133:LEU:HA	1:C:136:LYS:HB2	2.00	0.44
1:B:165:ARG:HD3	2:B:877:HOH:O	2.17	0.44
1:D:312:ARG:HD3	1:D:313:LYS:O	2.17	0.44
1:D:28:THR:OG1	1:D:29:LEU:N	2.47	0.44
1:C:110:LEU:O	1:C:113:PHE:HB3	2.17	0.44
1:A:139:ILE:HD12	1:A:141:CYS:SG	2.58	0.44
1:F:230:LEU:HD12	1:F:230:LEU:N	2.32	0.44
1:C:154:LEU:HD13	1:C:195:MET:HG2	1.99	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:N	1:E:90:GLU:OE1	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:HD12	1:C:133:LEU:N	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:E:154:LEU:CD1	1:E:195:MET:HB3	2.41	0.43
1:D:41:MET:HG3	1:D:72:GLU:HG2	2.00	0.43
1:C:67:GLY:O	1:C:68:LEU:C	2.55	0.43
1:E:246:LEU:HD22	1:E:250:GLN:HG3	2.00	0.43
1:C:78:SER:C	1:C:80:LYS:N	2.71	0.43
1:C:41:MET:CB	1:C:72:GLU:HG2	2.48	0.43
1:A:98:PHE:HB2	1:A:101:ILE:HD12	1.99	0.43
1:A:77:VAL:HG13	1:A:82:VAL:HG13	2.00	0.43
1:D:145:GLU:HA	1:D:148:GLN:OE1	2.17	0.43
1:C:206:ILE:HG13	1:C:208:VAL:HG13	1.99	0.43
1:F:279:GLU:HG2	1:F:300:LEU:HD23	2.00	0.43
1:F:184:LYS:HE3	1:F:188:VAL:CG2	2.48	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: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:140:ASN:HD22	1:D:140:ASN:HA	1.57	0.43
1:F:51:VAL:HB	1:F:55:VAL:HG11	2.01	0.43
1:E:270:GLN:CD	1:E:270:GLN:N	2.71	0.43
1:D:98:PHE:HB2	1:D:101:ILE:HD12	2.00	0.43
1:D:36:VAL:HG22	1:D:70:VAL:CG1	2.44	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:F:142:SER:HB3	1:F:145:GLU:CG	2.48	0.43
1:D:133:LEU:HB2	1:D:177:GLU:HG3	2.01	0.43
1:D:231:ALA:HB1	1:D:255:VAL:HG22	1.97	0.42
1:C:269:ALA:O	1:C:270:GLN:C	2.57	0.42
1:F:157:ALA:HB1	1:F:162:ILE:O	2.19	0.42
1:E:211:PRO:HG2	1:F:288:LEU:CD1	2.49	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:C:40:PRO:HA	1:C:44:LEU:CD2	2.40	0.42
1:B:232:VAL:HG22	1:B:234:CYS:SG	2.59	0.42
1:A:306:ILE:HG13	1:A:310:LEU:HD23	2.02	0.42
1:C:201:SER:HA	1:C:231:ALA:HB3	2.01	0.42
1:B:45:GLN:HG3	1:B:82:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:SG	1:B:175:PRO:HD2	2.60	0.42
1:C:90:GLU:HA	1:C:93:LYS:CE	2.50	0.42
1:A:43:GLY:HA2	1:A:264:GLY:HA3	2.02	0.42
1:C:205:THR:O	1:C:235:HIS:ND1	2.49	0.42
1:F:133:LEU:HD13	1:F:137:LYS:HZ3	1.84	0.42
1:D:278:THR:HG22	1:D:299:LEU:HD11	2.00	0.42
1:D:279:GLU:HG2	1:D:300:LEU:CD2	2.49	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: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:F:46:ASN:CB	1:F:265:GLY:H	2.33	0.41
1:E:226:PRO:O	1:E:230:LEU:CD2	2.68	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:B:111:LYS:O	1:B:114:GLU:HB3	2.18	0.41
1:A:139:ILE:O	1:A:141:CYS:N	2.53	0.41
1:D:279:GLU:HG3	1:D:299:LEU:HD13	2.02	0.41
1:C:37:GLU:OE2	1:C:260:VAL:N	2.48	0.41
1:E:106:LEU:N	1:E:106:LEU:HD12	2.35	0.41
1:E:41:MET:HG3	1:E:106:LEU:HD13	2.03	0.41
1:A:127:PHE:CD1	1:A:127:PHE:N	2.88	0.41
1:D:59:LEU:HD13	1:D:306:ILE:HB	2.02	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:78:SER:HA	1:A:79:PRO:HD3	1.94	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: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:C:139:ILE:HB	1:C:149:ARG:HH22	1.85	0.41
1:E:279:GLU:HB2	1:E:316:SER:OG	2.20	0.41
1:F:151:ASP:O	1:F:155:LYS:HB2	2.20	0.41
1:F:107:THR:HA	1:F:108:PRO:HD2	1.95	0.41
1:D:204:ASP:HA	2:D:615:HOH:O	2.20	0.41
1:D:41:MET:HB3	1:D:42:ASP:H	1.72	0.41
1:A:270:GLN:C	1:A:272:ALA:H	2.24	0.41
1:A:36:VAL:HG13	1:A:70:VAL:CG2	2.51	0.41
1:D:139:ILE:HG22	1:D:139:ILE:O	2.21	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:F:113:PHE:CD2	1:F:153:ILE:HG23	2.55	0.41
1:A:287:GLY:HA3	1:B:210:THR:HG21	2.02	0.41
1:D:53:THR:N	1:D:54:PRO:HD2	2.35	0.41
1:B:310:LEU:HA	1:B:310:LEU:HD12	1.96	0.41
1:C:139:ILE:HB	1:C:149:ARG:NH2	2.36	0.40
1:C:93:LYS:HB2	1:C:93:LYS:HE3	1.90	0.40
1:E:234:CYS:HB3	2:E:546:HOH:O	2.20	0.40
1:F:133:LEU:HD23	1:F:177:GLU:HG2	2.03	0.40
1:A:161:ASN:HA	1:A:161:ASN:HD22	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:E:133:LEU:O	1:E:137:LYS:HB2	2.21	0.40
1:D:113:PHE:O	1:D:117:VAL:HG23	2.21	0.40
1:C:174:CYS:SG	1:C:175:PRO:HD2	2.62	0.40
1:F:316:SER:O	1:F:320:GLN:HG3	2.21	0.40
1:A:151:ASP:O	1:A:155:LYS:HD3	2.22	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:F:288:LEU:HA	1:F:288:LEU:HD12	1.83	0.40
1:A:283:TYR:HB2	1:A:318:VAL:HG21	2.04	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%)	19	16
1	B	294/298 (99%)	281 (96%)	8 (3%)	5 (2%)	11	7
1	C	294/298 (99%)	271 (92%)	18 (6%)	5 (2%)	11	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	294/298 (99%)	280 (95%)	11 (4%)	3 (1%)	19	16
1	E	294/298 (99%)	282 (96%)	9 (3%)	3 (1%)	19	16
1	F	281/298 (94%)	258 (92%)	18 (6%)	5 (2%)	11	7
All	All	1751/1788 (98%)	1653 (94%)	74 (4%)	24 (1%)	14	10

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%)	16	16
1	B	238/240 (99%)	222 (93%)	16 (7%)	20	21
1	C	238/240 (99%)	223 (94%)	15 (6%)	22	24
1	D	238/240 (99%)	220 (92%)	18 (8%)	16	16
1	E	238/240 (99%)	222 (93%)	16 (7%)	20	21
1	F	231/240 (96%)	218 (94%)	13 (6%)	26	29
All	All	1421/1440 (99%)	1325 (93%)	96 (7%)	20	21

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

Some 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 carbohydrates 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%)	0.12	11 (3%) 45 44	20, 32, 54, 69	0
1	B	296/298 (99%)	0.50	26 (8%) 12 11	25, 40, 70, 84	0
1	C	296/298 (99%)	0.95	53 (17%) 2 2	31, 57, 76, 80	0
1	D	296/298 (99%)	0.40	29 (9%) 10 8	25, 38, 68, 79	0
1	E	296/298 (99%)	0.30	16 (5%) 29 29	26, 40, 62, 78	0
1	F	287/298 (96%)	1.17	71 (24%) 1 1	36, 58, 82, 88	0
All	All	1767/1788 (98%)	0.57	206 (11%) 6 6	20, 42, 74, 88	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	ILE	7.2
1	F	81	TRP	7.0
1	E	270	GLN	6.9
1	F	137	LYS	5.8
1	F	176	TYR	5.7
1	F	159	SER	5.7
1	F	110	LEU	5.5
1	C	152	ALA	5.4
1	C	118	ALA	5.3
1	C	50	ILE	5.2
1	F	114	GLU	5.0
1	F	134	PHE	4.9
1	C	160	ALA	4.9
1	C	48	LYS	4.8
1	F	157	ALA	4.7
1	B	50	ILE	4.5
1	F	38	VAL	4.4
1	C	147	PHE	4.4
1	B	140	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	160	ALA	4.4
1	C	161	ASN	4.3
1	C	270	GLN	4.3
1	B	48	LYS	4.3
1	B	138	ASN	4.2
1	F	80	LYS	4.2
1	B	323	CYS	4.1
1	F	272	ALA	4.1
1	F	133	LEU	4.0
1	B	141	CYS	4.0
1	D	83	PRO	4.0
1	F	51	VAL	3.9
1	B	147	PHE	3.9
1	E	323	CYS	3.9
1	D	270	GLN	3.9
1	D	323	CYS	3.9
1	A	270	GLN	3.8
1	C	155	LYS	3.8
1	F	136	LYS	3.8
1	F	82	VAL	3.8
1	A	268	TYR	3.8
1	B	81	TRP	3.7
1	C	271	GLY	3.7
1	E	322	THR	3.7
1	B	271	GLY	3.7
1	F	143	ILE	3.7
1	F	48	LYS	3.7
1	D	81	TRP	3.6
1	D	241	ALA	3.6
1	F	113	PHE	3.6
1	C	140	ASN	3.6
1	C	243	ALA	3.6
1	D	137	LYS	3.6
1	B	139	ILE	3.6
1	C	167	TYR	3.6
1	F	180	ILE	3.5
1	F	77	VAL	3.5
1	C	268	TYR	3.4
1	C	119	ALA	3.3
1	E	48	LYS	3.3
1	E	159	SER	3.3
1	B	36	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	311	ASN	3.3
1	C	81	TRP	3.3
1	D	243	ALA	3.3
1	D	140	ASN	3.3
1	F	233	HIS	3.2
1	F	49	ASN	3.2
1	F	258	SER	3.1
1	D	242	LEU	3.1
1	F	109	ASN	3.1
1	B	243	ALA	3.1
1	F	243	ALA	3.1
1	F	84	GLN	3.1
1	C	111	LYS	3.0
1	E	50	ILE	3.0
1	F	308	GLN	3.0
1	D	271	GLY	3.0
1	F	259	SER	3.0
1	C	120	GLY	3.0
1	B	270	GLN	3.0
1	C	112	GLY	2.9
1	C	269	ALA	2.9
1	E	243	ALA	2.9
1	C	141	CYS	2.9
1	C	110	LEU	2.9
1	F	276	LEU	2.9
1	F	323	CYS	2.9
1	B	260	VAL	2.9
1	C	195	MET	2.9
1	A	323	CYS	2.9
1	C	92	LEU	2.9
1	E	36	VAL	2.8
1	E	311	ASN	2.8
1	F	289	GLY	2.8
1	F	151	ASP	2.8
1	F	152	ALA	2.8
1	D	281	LEU	2.8
1	C	158	GLN	2.8
1	A	243	ALA	2.8
1	A	170	CYS	2.8
1	F	111	LYS	2.8
1	F	76	PHE	2.8
1	C	272	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	233	HIS	2.7
1	D	269	ALA	2.7
1	B	232	VAL	2.7
1	D	38	VAL	2.7
1	C	127	PHE	2.7
1	B	38	VAL	2.7
1	F	260	VAL	2.7
1	B	276	LEU	2.7
1	F	275	ASN	2.7
1	F	162	ILE	2.6
1	D	268	TYR	2.6
1	F	234	CYS	2.6
1	F	120	GLY	2.6
1	F	179	LYS	2.6
1	D	110	LEU	2.6
1	F	83	PRO	2.6
1	D	260	VAL	2.6
1	D	276	LEU	2.6
1	F	148	GLN	2.6
1	C	156	ALA	2.6
1	F	241	ALA	2.6
1	C	71	ILE	2.6
1	D	82	VAL	2.5
1	C	95	ILE	2.5
1	F	112	GLY	2.5
1	D	133	LEU	2.5
1	D	322	THR	2.5
1	F	135	THR	2.5
1	B	148	GLN	2.5
1	F	291	HIS	2.5
1	A	266	CYS	2.5
1	C	148	GLN	2.5
1	F	128	GLY	2.5
1	C	114	GLU	2.5
1	E	148	GLN	2.5
1	D	234	CYS	2.5
1	E	258	SER	2.5
1	D	267	PRO	2.5
1	F	130	ALA	2.4
1	C	154	LEU	2.4
1	C	49	ASN	2.4
1	C	232	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	260	VAL	2.4
1	E	271	GLY	2.4
1	B	70	VAL	2.4
1	F	154	LEU	2.4
1	F	155	LYS	2.4
1	A	276	LEU	2.3
1	F	36	VAL	2.3
1	B	118	ALA	2.3
1	C	258	SER	2.3
1	A	48	LYS	2.3
1	F	71	ILE	2.3
1	F	235	HIS	2.3
1	D	255	VAL	2.2
1	F	185	VAL	2.2
1	D	308	GLN	2.2
1	F	242	LEU	2.2
1	D	272	ALA	2.2
1	D	232	VAL	2.2
1	F	311	ASN	2.2
1	C	139	ILE	2.2
1	C	313	LYS	2.2
1	F	167	TYR	2.2
1	B	144	GLU	2.2
1	F	144	GLU	2.2
1	F	115	ALA	2.2
1	E	38	VAL	2.2
1	B	201	SER	2.2
1	C	159	SER	2.2
1	C	241	ALA	2.2
1	D	156	ALA	2.2
1	B	322	THR	2.1
1	C	151	ASP	2.1
1	F	297	GLN	2.1
1	C	125	VAL	2.1
1	E	70	VAL	2.1
1	E	49	ASN	2.1
1	C	242	LEU	2.1
1	C	166	GLY	2.1
1	F	78	SER	2.1
1	C	133	LEU	2.1
1	F	119	ALA	2.1
1	F	201	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	257	ASP	2.1
1	A	271	GLY	2.1
1	A	269	ALA	2.1
1	B	152	ALA	2.1
1	F	116	ALA	2.1
1	F	158	GLN	2.1
1	A	260	VAL	2.1
1	F	161	ASN	2.0
1	C	162	ILE	2.0
1	B	241	ALA	2.0
1	C	234	CYS	2.0
1	C	307	CYS	2.0
1	F	238	TYR	2.0
1	D	258	SER	2.0
1	C	80	LYS	2.0
1	C	28	THR	2.0
1	C	322	THR	2.0
1	B	269	ALA	2.0
1	E	269	ALA	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 carbohydrates 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.