



Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2016 – 07:39 AM EDT

PDB ID : 5CBQ
Title : Crystal structure of a T1-like thiolase from Mycobacterium smegmatis
Authors : Janardan, N.; Murthy, M.R.N.
Deposited on : 2015-07-01
Resolution : 2.45 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

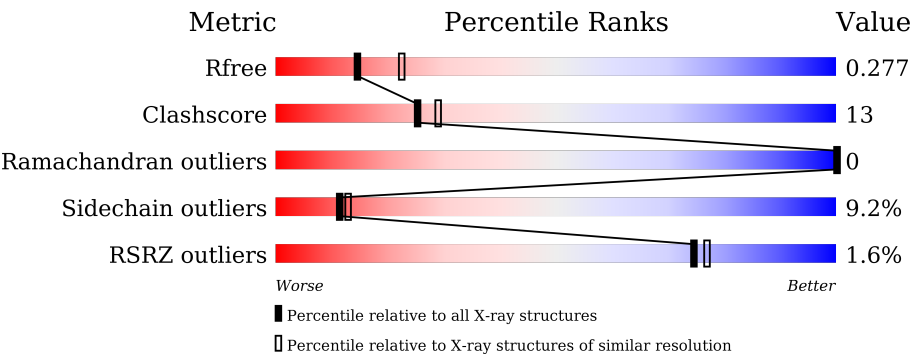
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	413	<div><div>3%</div><div><div></div><div>71%</div><div>23%</div><div></div></div><div></div></div>
1	B	413	<div><div></div><div><div></div><div>71%</div><div>21%</div><div></div></div><div></div></div>
1	C	413	<div><div>%</div><div><div></div><div>71%</div><div>22%</div><div></div></div><div></div></div>
1	D	413	<div><div></div><div><div></div><div>72%</div><div>23%</div><div></div></div><div></div></div>
1	E	413	<div><div>%</div><div><div></div><div>75%</div><div>20%</div><div></div></div><div></div></div>
1	F	413	<div><div>5%</div><div><div></div><div>68%</div><div>23%</div><div></div></div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17727 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 Beta-ketothiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			2868	1770	525	557	16			
1	B	398	Total	C	N	O	S	0	2	0
			2943	1823	538	566	16			
1	C	397	Total	C	N	O	S	0	0	0
			2882	1786	522	558	16			
1	D	398	Total	C	N	O	S	0	1	0
			2927	1813	535	563	16			
1	E	400	Total	C	N	O	S	0	0	0
			2925	1811	538	560	16			
1	F	393	Total	C	N	O	S	0	0	0
			2846	1763	523	544	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP A0QUH3
A	-4	HIS	-	expression tag	UNP A0QUH3
A	-3	HIS	-	expression tag	UNP A0QUH3
A	-2	HIS	-	expression tag	UNP A0QUH3
A	-1	HIS	-	expression tag	UNP A0QUH3
A	0	HIS	-	expression tag	UNP A0QUH3
B	-5	HIS	-	expression tag	UNP A0QUH3
B	-4	HIS	-	expression tag	UNP A0QUH3
B	-3	HIS	-	expression tag	UNP A0QUH3
B	-2	HIS	-	expression tag	UNP A0QUH3
B	-1	HIS	-	expression tag	UNP A0QUH3
B	0	HIS	-	expression tag	UNP A0QUH3
C	-5	HIS	-	expression tag	UNP A0QUH3
C	-4	HIS	-	expression tag	UNP A0QUH3
C	-3	HIS	-	expression tag	UNP A0QUH3
C	-2	HIS	-	expression tag	UNP A0QUH3
C	-1	HIS	-	expression tag	UNP A0QUH3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0QUH3
D	-5	HIS	-	expression tag	UNP A0QUH3
D	-4	HIS	-	expression tag	UNP A0QUH3
D	-3	HIS	-	expression tag	UNP A0QUH3
D	-2	HIS	-	expression tag	UNP A0QUH3
D	-1	HIS	-	expression tag	UNP A0QUH3
D	0	HIS	-	expression tag	UNP A0QUH3
E	-5	HIS	-	expression tag	UNP A0QUH3
E	-4	HIS	-	expression tag	UNP A0QUH3
E	-3	HIS	-	expression tag	UNP A0QUH3
E	-2	HIS	-	expression tag	UNP A0QUH3
E	-1	HIS	-	expression tag	UNP A0QUH3
E	0	HIS	-	expression tag	UNP A0QUH3
F	-5	HIS	-	expression tag	UNP A0QUH3
F	-4	HIS	-	expression tag	UNP A0QUH3
F	-3	HIS	-	expression tag	UNP A0QUH3
F	-2	HIS	-	expression tag	UNP A0QUH3
F	-1	HIS	-	expression tag	UNP A0QUH3
F	0	HIS	-	expression tag	UNP A0QUH3

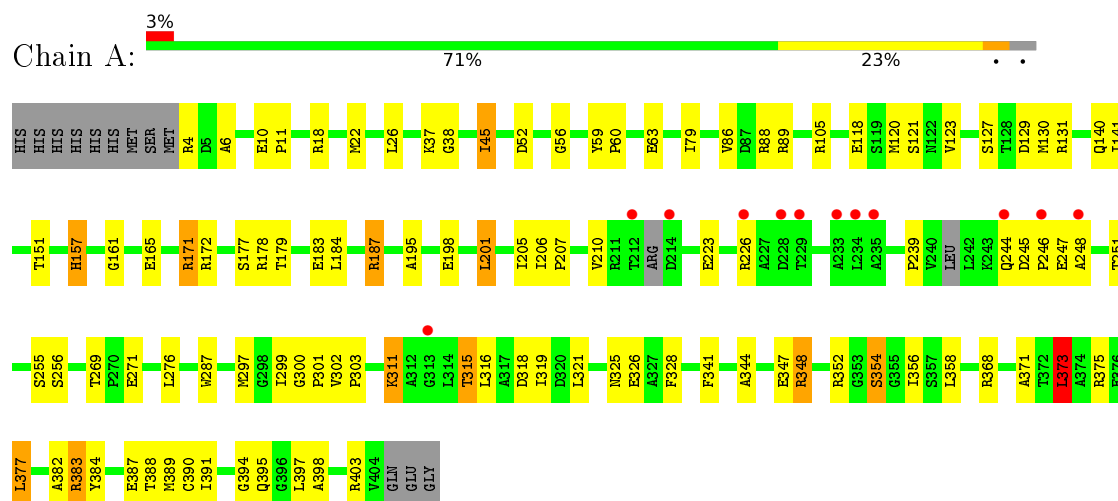
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	51	Total O 51 51	0	0
2	B	66	Total O 66 66	0	0
2	C	55	Total O 55 55	0	0
2	D	69	Total O 69 69	0	0
2	E	49	Total O 49 49	0	0
2	F	46	Total O 46 46	0	0

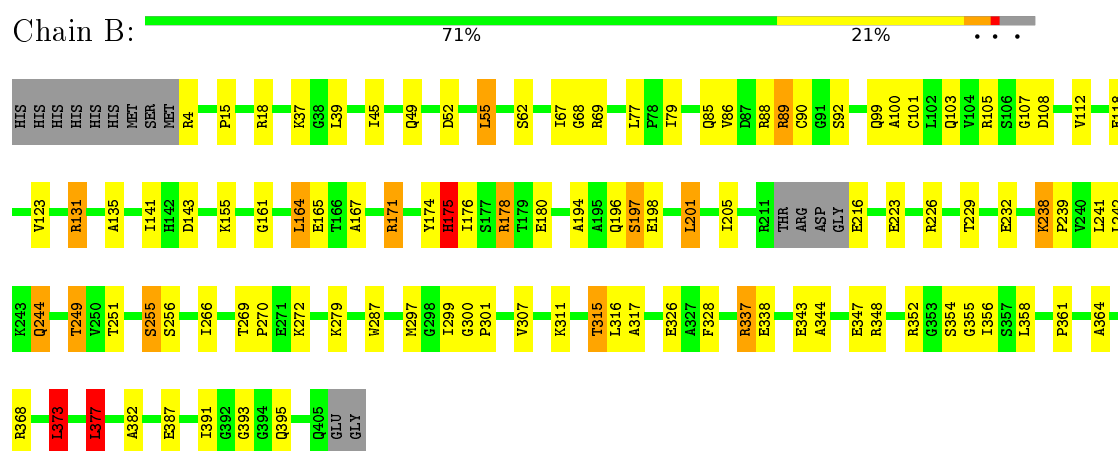
3 Residue-property plots

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.

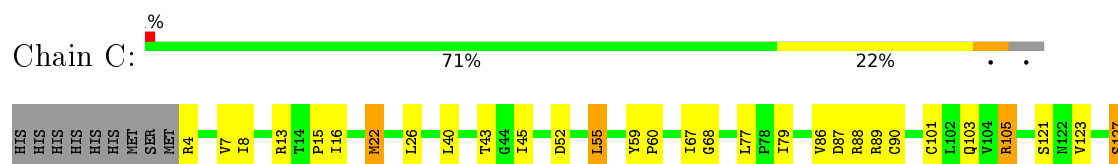
• Molecule 1: Beta-ketothiolase

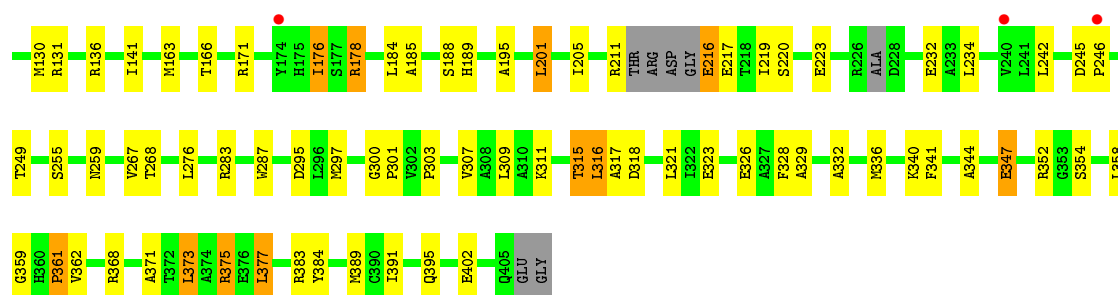


• Molecule 1: Beta-ketothiolase



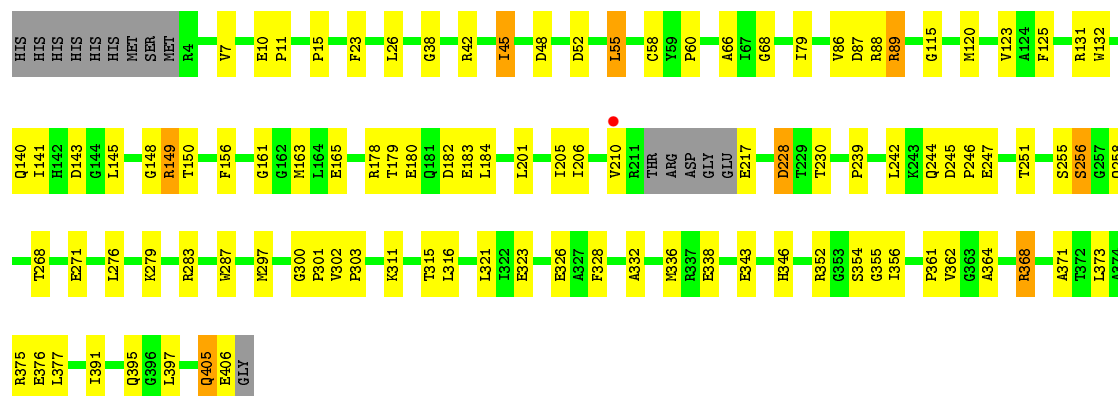
• Molecule 1: Beta-ketothiolase





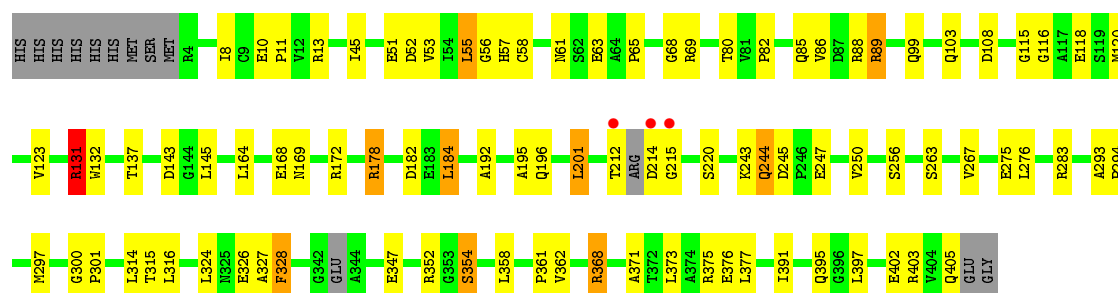
• Molecule 1: Beta-ketothiolase

Chain D: 72% 23% . .



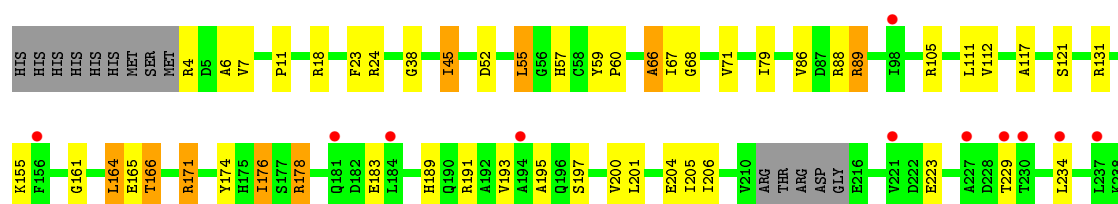
• Molecule 1: Beta-ketothiolase

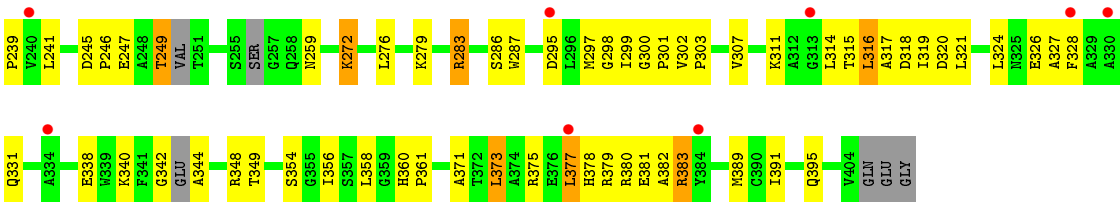
Chain E: % 75% 20% . .



• Molecule 1: Beta-ketothiolase

Chain F: 5% 68% 23% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.46Å 181.47Å 271.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	135.87 – 2.45 52.35 – 2.45	Depositor EDS
% Data completeness (in resolution range)	89.1 (135.87-2.45) 89.1 (52.35-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.226 , 0.268 0.225 , 0.277	Depositor DCC
R_{free} test set	4603 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17727	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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	1.39	3/2911 (0.1%)	0.89	2/3957 (0.1%)
1	B	1.54	7/2991 (0.2%)	0.96	6/4058 (0.1%)
1	C	1.38	0/2925	0.88	4/3974 (0.1%)
1	D	1.48	3/2971 (0.1%)	0.94	6/4033 (0.1%)
1	E	1.34	4/2968 (0.1%)	0.89	2/4028 (0.0%)
1	F	1.22	0/2886	0.86	1/3915 (0.0%)
All	All	1.40	17/17652 (0.1%)	0.91	21/23965 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
All	All	0	7

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	GLU	CD-OE1	-6.23	1.18	1.25
1	B	175[A]	HIS	N-CA	6.12	1.58	1.46
1	B	175[B]	HIS	N-CA	6.12	1.58	1.46
1	E	118	GLU	CD-OE2	-5.71	1.19	1.25
1	A	118	GLU	CD-OE2	-5.64	1.19	1.25
1	E	132	TRP	CB-CG	-5.63	1.40	1.50
1	B	393	GLY	C-O	-5.62	1.14	1.23
1	D	338	GLU	CD-OE2	-5.56	1.19	1.25
1	D	323	GLU	CD-OE2	-5.54	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	GLU	CD-OE2	-5.50	1.19	1.25
1	B	174	TYR	CE1-CZ	-5.41	1.31	1.38
1	B	118	GLU	CD-OE2	-5.38	1.19	1.25
1	A	63	GLU	CD-OE1	-5.33	1.19	1.25
1	E	376	GLU	CD-OE1	-5.28	1.19	1.25
1	B	338	GLU	CD-OE1	-5.25	1.19	1.25
1	A	56	GLY	C-O	-5.24	1.15	1.23
1	D	323	GLU	CD-OE1	-5.17	1.20	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197[A]	SER	C-N-CA	12.34	152.56	121.70
1	B	197[B]	SER	C-N-CA	12.34	152.56	121.70
1	D	149[A]	ARG	C-N-CA	7.74	141.05	121.70
1	D	149[B]	ARG	C-N-CA	7.74	141.05	121.70
1	D	148	GLY	CA-C-N	7.16	132.96	117.20
1	B	174	TYR	C-N-CA	7.00	139.19	121.70
1	C	87	ASP	CB-CG-OD1	6.58	124.22	118.30
1	D	148	GLY	O-C-N	-6.56	112.21	122.70
1	B	373	LEU	CA-CB-CG	6.33	129.85	115.30
1	E	131	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	375	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	129	ASP	CB-CG-OD2	5.85	123.57	118.30
1	E	69	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	373	LEU	CA-CB-CG	5.58	128.15	115.30
1	B	377	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	373	LEU	CA-CB-CG	5.38	127.69	115.30
1	B	90	CYS	CB-CA-C	5.32	121.05	110.40
1	C	13	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	F	373	LEU	CA-CB-CG	5.13	127.09	115.30
1	D	87	ASP	CB-CG-OD1	5.02	122.82	118.30
1	D	48	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	PRO	Peptide
1	C	361	PRO	Peptide
1	D	361	PRO	Peptide
1	D	66	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	E	361	PRO	Peptide
1	F	361	PRO	Peptide
1	F	66	ALA	Peptide

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	A	2868	0	2782	89	0
1	B	2943	0	2941	83	0
1	C	2882	0	2840	89	0
1	D	2927	0	2917	73	0
1	E	2925	0	2912	72	0
1	F	2846	0	2799	76	0
2	A	51	0	0	3	0
2	B	66	0	0	6	0
2	C	55	0	0	2	0
2	D	69	0	0	4	0
2	E	49	0	0	1	0
2	F	46	0	0	2	0
All	All	17727	0	17191	437	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 13.

All (437) 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:A:131:ARG:NH2	1:B:143:ASP:OD1	1.60	1.35
1:E:108:ASP:OD1	1:F:311:LYS:NZ	1.75	1.18
1:A:131:ARG:NH1	1:B:123:VAL:O	1.78	1.15
1:A:141:ILE:HD11	1:D:141:ILE:HD11	1.27	1.08
1:B:326:GLU:OE1	1:B:354:SER:HB3	1.56	1.05
1:E:86:VAL:HG12	1:F:86:VAL:HG12	1.39	1.03
1:D:326:GLU:OE1	1:D:354:SER:HB3	1.57	1.02
1:A:344:ALA:O	1:A:347:GLU:HB2	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLN:OE1	1:B:272:LYS:NZ	1.93	1.00
1:C:326:GLU:OE1	1:C:354:SER:HB3	1.61	0.98
1:F:176:ILE:HD12	1:F:176:ILE:H	1.28	0.98
1:B:141:ILE:HD11	1:C:141:ILE:CD1	1.94	0.96
1:B:141:ILE:HD11	1:C:141:ILE:HD11	1.46	0.96
1:F:11:PRO:O	1:F:375:ARG:NH1	1.97	0.96
1:B:251:THR:O	1:B:255:SER:OG	1.81	0.96
1:E:358:LEU:HD13	1:E:368:ARG:NH1	1.82	0.94
1:C:131:ARG:NH2	1:D:143:ASP:OD1	2.02	0.92
1:E:212:THR:C	1:E:215:GLY:O	2.08	0.92
1:E:358:LEU:CD1	1:E:368:ARG:NH1	2.33	0.91
1:A:86:VAL:HG12	1:B:86:VAL:HG12	1.52	0.91
1:A:141:ILE:HD11	1:D:141:ILE:CD1	2.01	0.89
1:B:18:ARG:HG3	1:B:223:GLU:HG2	1.53	0.88
1:C:245:ASP:OD1	1:C:246:PRO:HD2	1.75	0.87
1:E:212:THR:C	1:E:214:ASP:N	2.28	0.86
1:C:45:ILE:CD1	1:C:276:LEU:HD13	2.06	0.86
1:E:88:ARG:NH2	1:F:52:ASP:OD1	2.09	0.86
1:B:39:LEU:HD11	1:B:266:ILE:HD12	1.58	0.85
1:F:189:HIS:O	1:F:193:VAL:HG23	1.77	0.84
1:C:163:MET:O	1:C:166:THR:OG1	1.96	0.82
1:F:171:ARG:CG	1:F:176:ILE:HD13	1.97	0.82
1:F:315:THR:O	1:F:318:ASP:HB2	1.79	0.82
1:A:88:ARG:NH2	1:B:52:ASP:OD1	2.13	0.82
1:A:383:ARG:HD3	1:A:384:TYR:CE2	2.15	0.81
1:F:171:ARG:HG2	1:F:176:ILE:HD13	1.61	0.81
1:E:123:VAL:O	1:F:131:ARG:NH1	2.14	0.81
1:D:55:LEU:HD22	1:D:68:GLY:HA2	1.62	0.81
1:F:326:GLU:CD	1:F:354:SER:HB3	2.02	0.80
1:A:184:LEU:HA	1:A:187:ARG:NH1	1.97	0.79
1:B:141:ILE:CD1	1:C:141:ILE:HD11	2.12	0.79
1:C:55:LEU:HD22	1:C:68:GLY:HA2	1.65	0.79
1:E:55:LEU:HD22	1:E:68:GLY:HA2	1.64	0.79
1:B:344:ALA:O	1:B:347:GLU:HB2	1.83	0.78
1:C:45:ILE:HD11	1:C:276:LEU:HD13	1.66	0.78
1:E:212:THR:O	1:E:215:GLY:O	2.00	0.78
1:E:245:ASP:OD1	1:E:247:GLU:N	2.17	0.78
1:B:141:ILE:CD1	1:C:141:ILE:CD1	2.63	0.77
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.50	0.77
1:C:344:ALA:O	1:C:347:GLU:HB2	1.85	0.76
1:B:171:ARG:HA	1:B:176:ILE:HD12	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ILE:HB	1:C:395:GLN:HB2	1.66	0.76
1:C:245:ASP:OD1	1:C:246:PRO:CD	2.34	0.76
1:B:178:ARG:HB2	1:B:249:THR:HG22	1.67	0.75
1:E:143:ASP:OD1	1:F:131:ARG:NH2	2.20	0.75
1:F:326:GLU:OE1	1:F:354:SER:HB3	1.87	0.75
1:C:22:MET:SD	1:C:223:GLU:HB2	2.27	0.74
1:E:358:LEU:HD13	1:E:368:ARG:HH11	1.51	0.74
1:A:171:ARG:NH1	1:A:247:GLU:O	2.21	0.74
1:F:55:LEU:HD22	1:F:68:GLY:HA2	1.68	0.74
1:B:55:LEU:HD22	1:B:68:GLY:HA2	1.68	0.74
1:A:171:ARG:HD2	1:A:172:ARG:N	2.04	0.72
1:A:171:ARG:HD2	1:A:171:ARG:C	2.10	0.71
1:C:131:ARG:HH22	1:D:143:ASP:CG	1.93	0.71
1:B:337:ARG:HG2	1:B:337:ARG:HH11	1.57	0.70
1:D:15:PRO:HD3	1:D:205:ILE:HG23	1.72	0.70
1:C:131:ARG:NH1	1:D:123:VAL:O	2.25	0.70
1:B:326:GLU:CD	1:B:354:SER:HB3	2.12	0.70
1:F:164:LEU:HD22	1:F:328:PHE:HE2	1.56	0.70
1:C:45:ILE:HD12	1:C:276:LEU:HD13	1.74	0.69
1:B:141:ILE:HD11	1:C:141:ILE:HD12	1.73	0.69
1:C:89:ARG:HB2	1:C:391:ILE:HG23	1.74	0.69
1:F:176:ILE:CD1	1:F:176:ILE:H	2.02	0.69
1:B:391:ILE:HB	1:B:395:GLN:HB2	1.75	0.69
1:F:326:GLU:HB3	1:F:356:ILE:HD12	1.74	0.69
1:B:326:GLU:HB3	1:B:356:ILE:HD12	1.74	0.68
1:E:212:THR:CA	1:E:215:GLY:O	2.42	0.68
1:A:45:ILE:HD11	1:A:276:LEU:HB3	1.75	0.68
1:E:184:LEU:HD11	1:E:326:GLU:OE2	1.93	0.68
1:C:255:SER:HB2	1:C:328:PHE:CD1	2.29	0.68
1:A:187:ARG:NH1	1:A:187:ARG:HG3	2.06	0.67
1:A:371:ALA:O	1:A:375:ARG:HG3	1.93	0.67
1:C:287:TRP:O	1:C:311:LYS:CE	2.42	0.67
1:F:321:LEU:HD12	1:F:377:LEU:CD1	2.25	0.67
1:B:337:ARG:CG	1:B:337:ARG:HH11	2.07	0.67
1:D:256:SER:HB3	1:D:355:GLY:O	1.94	0.67
1:E:123:VAL:HG21	1:E:145:LEU:HD21	1.75	0.67
1:E:168:GLU:OE2	1:E:250:VAL:HG23	1.94	0.67
1:C:315:THR:HG22	1:C:317:ALA:H	1.59	0.67
1:D:245:ASP:OD1	1:D:247:GLU:N	2.25	0.67
1:B:135:ALA:HB2	1:D:131:ARG:O	1.95	0.66
1:D:45:ILE:HD11	1:D:276:LEU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:HD2	2:B:514:HOH:O	1.95	0.66
1:C:131:ARG:NH2	1:D:143:ASP:CG	2.47	0.66
1:A:89:ARG:HB2	1:A:391:ILE:HG23	1.76	0.66
1:C:321:LEU:HD12	1:C:377:LEU:CD1	2.26	0.66
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.59	0.65
1:A:201:LEU:O	1:A:205:ILE:HG12	1.95	0.65
1:E:371:ALA:O	1:E:375:ARG:HG3	1.96	0.65
1:B:287:TRP:O	1:B:311:LYS:HE3	1.96	0.65
1:F:176:ILE:N	1:F:176:ILE:HD12	2.07	0.65
1:F:45:ILE:HD11	1:F:276:LEU:HB3	1.77	0.65
1:B:196:GLN:HG3	1:B:201:LEU:HD23	1.77	0.65
1:D:326:GLU:OE1	1:D:354:SER:CB	2.39	0.65
1:F:315:THR:HG22	1:F:317:ALA:H	1.59	0.65
1:A:161:GLY:HA3	1:A:165:GLU:OE1	1.96	0.65
1:E:326:GLU:OE1	1:E:354:SER:HB3	1.97	0.65
1:C:22:MET:HG2	1:C:219:ILE:HD13	1.79	0.64
1:A:52:ASP:OD1	1:B:88:ARG:NH2	2.31	0.64
1:F:178:ARG:HB2	1:F:249:THR:HG22	1.80	0.64
1:B:88:ARG:N	1:B:92:SER:OG	2.27	0.63
1:A:358:LEU:HD13	1:A:368:ARG:NH1	2.13	0.63
1:A:187:ARG:HH11	1:A:187:ARG:CG	2.11	0.63
1:A:319:ILE:O	1:A:348:ARG:NH1	2.31	0.63
1:C:121:SER:O	1:D:131:ARG:HD3	1.99	0.62
1:F:298:GLY:HA3	1:F:331:GLN:HG2	1.81	0.62
1:C:383:ARG:HD3	1:C:384:TYR:CE2	2.35	0.62
1:E:192:ALA:O	1:E:196:GLN:HG3	2.00	0.62
1:E:89:ARG:HB2	1:E:391:ILE:HG23	1.81	0.62
1:B:4:ARG:N	2:B:505:HOH:O	2.32	0.62
1:C:88:ARG:NH2	1:D:52:ASP:OD1	2.33	0.61
1:A:358:LEU:CD1	1:A:368:ARG:NH1	2.64	0.61
1:E:13:ARG:HD3	1:E:368:ARG:HG3	1.81	0.61
1:A:300:GLY:N	1:A:301:PRO:HD2	2.14	0.61
1:A:255:SER:HB2	1:A:328:PHE:CD1	2.35	0.61
1:E:391:ILE:HB	1:E:395:GLN:HB2	1.81	0.61
1:D:7:VAL:HG12	1:D:283:ARG:HB3	1.81	0.61
1:C:127:SER:HB3	1:C:130:MET:HG3	1.83	0.61
1:D:149[A]:ARG:NH2	1:D:258:GLN:OE1	2.34	0.61
1:E:212:THR:N	1:E:215:GLY:O	2.33	0.61
1:C:326:GLU:CD	1:C:354:SER:HB3	2.21	0.60
1:F:45:ILE:HD11	1:F:276:LEU:CB	2.31	0.60
1:B:255:SER:HB3	1:B:328:PHE:HD1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:CYS:SG	1:D:362:VAL:HG12	2.42	0.60
1:A:377:LEU:HD12	1:A:382:ALA:HB3	1.84	0.59
1:A:38:GLY:HA3	1:A:206:ILE:HD12	1.83	0.59
1:E:99:GLN:O	1:E:103:GLN:HG3	2.02	0.59
1:A:161:GLY:HA3	1:A:165:GLU:HB2	1.84	0.59
1:B:377:LEU:HD12	1:B:382:ALA:HB3	1.85	0.59
1:C:178:ARG:NH1	1:C:234:LEU:O	2.36	0.59
1:F:391:ILE:HB	1:F:395:GLN:HB2	1.85	0.59
1:C:178:ARG:HB2	1:C:249:THR:HG22	1.85	0.58
1:A:88:ARG:HH22	1:B:52:ASP:CG	2.04	0.58
1:F:342:GLY:O	1:F:344:ALA:N	2.37	0.58
1:A:287:TRP:O	1:A:311:LYS:HE2	2.03	0.58
1:F:321:LEU:HD12	1:F:377:LEU:HD12	1.84	0.58
1:C:287:TRP:O	1:C:311:LYS:HE3	2.04	0.58
1:F:298:GLY:CA	1:F:331:GLN:HG2	2.33	0.58
1:D:391:ILE:HB	1:D:395:GLN:HB2	1.85	0.57
1:D:405:GLN:HA	1:D:405:GLN:NE2	2.20	0.57
1:C:255:SER:HB2	1:C:328:PHE:HD1	1.68	0.57
1:C:171:ARG:HA	1:C:176:ILE:HG13	1.85	0.57
1:B:89:ARG:HB2	1:B:391:ILE:HG23	1.86	0.57
1:C:184:LEU:HD23	1:C:329:ALA:HB1	1.87	0.57
1:B:161:GLY:HA3	1:B:165:GLU:OE1	2.05	0.56
1:C:123:VAL:O	1:D:131:ARG:NH1	2.37	0.56
1:D:89:ARG:HB2	1:D:391:ILE:HG23	1.86	0.56
1:F:383:ARG:HG3	1:F:383:ARG:NH1	2.18	0.56
1:C:242:LEU:HA	1:C:245:ASP:O	2.06	0.56
1:C:315:THR:HG22	1:C:317:ALA:N	2.21	0.56
1:F:67:ILE:O	1:F:71:VAL:HG23	2.04	0.56
1:C:88:ARG:HH22	1:D:52:ASP:CG	2.08	0.56
1:B:232:GLU:CD	1:B:232:GLU:H	2.09	0.56
1:F:178:ARG:NH2	1:F:239:PRO:HD3	2.20	0.56
1:D:11:PRO:O	1:D:375:ARG:NH1	2.39	0.56
1:D:332:ALA:O	1:D:336:MET:HG3	2.05	0.56
1:D:364:ALA:HA	2:D:525:HOH:O	2.06	0.55
1:F:300:GLY:N	1:F:301:PRO:CD	2.68	0.55
1:A:179:THR:O	1:A:183:GLU:HG3	2.06	0.55
1:C:232:GLU:N	1:C:232:GLU:OE1	2.38	0.55
1:D:123:VAL:HG21	1:D:145:LEU:HD21	1.89	0.55
1:C:195:ALA:HB2	1:C:352:ARG:HD2	1.88	0.55
1:A:121:SER:O	1:B:131:ARG:HD3	2.07	0.55
1:A:321:LEU:HD12	1:A:377:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ARG:HH22	1:F:52:ASP:CG	2.09	0.55
1:A:207:PRO:HD2	2:A:544:HOH:O	2.07	0.54
1:A:391:ILE:HB	1:A:395:GLN:HB2	1.88	0.54
1:C:211:ARG:HA	1:C:216:GLU:HG2	1.89	0.54
1:A:131:ARG:NH2	1:B:143:ASP:CG	2.52	0.54
1:C:163:MET:N	2:C:503:HOH:O	2.39	0.54
1:A:171:ARG:NH1	1:A:171:ARG:HG3	2.22	0.54
1:B:18:ARG:CG	1:B:223:GLU:HG2	2.34	0.54
1:B:178:ARG:NH2	1:B:239:PRO:HD3	2.21	0.54
1:C:321:LEU:HD12	1:C:377:LEU:HD13	1.87	0.54
1:E:13:ARG:HD3	1:E:368:ARG:CG	2.37	0.54
1:E:8:ILE:HD12	1:E:267:VAL:HG22	1.88	0.54
1:E:13:ARG:CD	1:E:368:ARG:HG3	2.37	0.54
1:D:287:TRP:O	1:D:311:LYS:HE3	2.07	0.54
1:E:52:ASP:OD1	1:F:88:ARG:NH2	2.40	0.54
1:A:4:ARG:O	1:A:105:ARG:HG2	2.08	0.54
1:A:245:ASP:OD1	1:A:247:GLU:N	2.30	0.54
1:E:168:GLU:CD	1:E:250:VAL:HG23	2.28	0.54
1:E:212:THR:O	1:E:214:ASP:N	2.40	0.54
1:B:15:PRO:HD3	1:B:205:ILE:HG23	1.91	0.53
1:A:120:MET:HA	1:A:123:VAL:HG23	1.89	0.53
1:A:383:ARG:HD3	1:A:384:TYR:CZ	2.42	0.53
1:E:328:PHE:CD1	1:E:328:PHE:N	2.77	0.53
1:A:239:PRO:HG2	1:A:248:ALA:O	2.08	0.53
1:A:344:ALA:O	1:A:347:GLU:CB	2.44	0.53
1:A:326:GLU:OE1	1:A:354:SER:HB3	2.09	0.53
1:A:172:ARG:NH1	1:A:245:ASP:OD2	2.41	0.53
1:E:184:LEU:HD12	1:E:184:LEU:C	2.28	0.53
1:F:7:VAL:HG12	1:F:283:ARG:HB2	1.90	0.53
1:A:315:THR:O	1:A:318:ASP:HB2	2.09	0.53
1:B:315:THR:HG23	1:B:317:ALA:H	1.73	0.53
1:C:242:LEU:O	1:C:245:ASP:O	2.27	0.53
1:E:120:MET:HA	1:E:123:VAL:HG23	1.91	0.53
1:C:315:THR:O	1:C:318:ASP:HB2	2.09	0.53
1:C:371:ALA:O	1:C:375:ARG:HG3	2.09	0.53
1:D:178:ARG:HH21	1:D:239:PRO:HG3	1.74	0.53
1:B:175[B]:HIS:ND1	2:B:501:HOH:O	2.37	0.52
1:C:332:ALA:O	1:C:336:MET:HG3	2.09	0.52
1:D:255:SER:HB2	1:D:328:PHE:CD1	2.44	0.52
1:D:23:PHE:HB2	2:D:516:HOH:O	2.09	0.52
1:A:311:LYS:NZ	1:B:108:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:THR:HB	1:B:270:PRO:CD	2.40	0.52
1:E:58:CYS:SG	1:E:362:VAL:HG12	2.48	0.52
1:E:86:VAL:HG12	1:F:86:VAL:CG1	2.26	0.52
1:B:161:GLY:HA3	1:B:165:GLU:HB2	1.91	0.52
1:C:300:GLY:N	1:C:301:PRO:CD	2.73	0.52
1:D:10:GLU:OE2	1:D:42:ARG:NH1	2.41	0.52
1:E:327:ALA:C	1:E:328:PHE:CD1	2.84	0.52
1:A:302:VAL:HB	1:A:303:PRO:CD	2.41	0.51
1:C:52:ASP:OD1	1:D:88:ARG:NH2	2.43	0.51
1:E:131:ARG:HD3	1:F:121:SER:O	2.09	0.51
1:B:99:GLN:O	1:B:103:GLN:HG3	2.10	0.51
1:B:141:ILE:CD1	1:C:141:ILE:HD12	2.34	0.51
1:C:344:ALA:O	1:C:347:GLU:N	2.37	0.51
1:D:179:THR:O	1:D:183:GLU:HB2	2.10	0.51
1:B:373:LEU:O	1:B:377:LEU:HB2	2.10	0.51
1:F:204:GLU:HG2	1:F:371:ALA:HB1	1.93	0.51
1:E:300:GLY:N	1:E:301:PRO:CD	2.74	0.51
1:E:65:PRO:HB3	1:F:89:ARG:NH1	2.26	0.51
1:B:194:ALA:O	1:B:198:GLU:HB2	2.10	0.50
1:F:279:LYS:O	1:F:279:LYS:HG2	2.12	0.50
1:D:178:ARG:HD2	1:D:182:ASP:OD2	2.12	0.50
1:F:321:LEU:HD12	1:F:377:LEU:HD13	1.93	0.50
1:A:161:GLY:CA	1:A:165:GLU:OE1	2.59	0.50
1:B:238:LYS:HG2	1:B:238:LYS:O	2.12	0.50
1:D:228:ASP:O	1:D:230:THR:HG23	2.11	0.50
1:D:245:ASP:OD1	1:D:247:GLU:HB2	2.12	0.50
1:E:184:LEU:HD12	1:E:184:LEU:O	2.12	0.50
1:F:57:HIS:ND1	1:F:117:ALA:O	2.37	0.50
1:A:127:SER:HB3	1:A:130:MET:HG3	1.94	0.49
1:C:391:ILE:HB	1:C:395:GLN:CB	2.40	0.49
1:E:326:GLU:OE1	1:E:354:SER:CB	2.59	0.49
1:B:239:PRO:HA	1:B:251:THR:HG22	1.93	0.49
1:B:354:SER:OG	1:B:355:GLY:N	2.46	0.49
1:A:195:ALA:HB2	1:A:352:ARG:HD2	1.94	0.49
1:E:354:SER:O	1:E:358:LEU:HB2	2.12	0.49
1:C:101:CYS:O	1:C:105:ARG:HG3	2.13	0.49
1:D:38:GLY:HA3	1:D:206:ILE:HD12	1.95	0.49
1:D:271:GLU:CD	1:D:271:GLU:H	2.15	0.49
1:A:171:ARG:HH21	1:A:172:ARG:NH1	2.10	0.49
1:A:89:ARG:HB2	1:A:391:ILE:CG2	2.42	0.49
1:C:16:ILE:HG23	1:C:361:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:THR:HG22	1:C:295:ASP:O	2.12	0.49
1:A:358:LEU:HD13	1:A:368:ARG:HH11	1.78	0.49
1:A:383:ARG:CD	1:A:384:TYR:CE2	2.93	0.49
1:C:358:LEU:HD13	1:C:368:ARG:HD2	1.94	0.49
1:F:383:ARG:HG3	1:F:383:ARG:HH11	1.78	0.49
1:C:321:LEU:HD12	1:C:377:LEU:HD12	1.93	0.48
1:E:195:ALA:HB2	1:E:352:ARG:HD2	1.94	0.48
1:F:320:ASP:CB	1:F:382:ALA:HB1	2.43	0.48
1:A:161:GLY:HA3	1:A:165:GLU:CB	2.43	0.48
1:D:149[B]:ARG:HG2	1:D:163:MET:HG2	1.94	0.48
1:C:287:TRP:O	1:C:311:LYS:NZ	2.46	0.48
1:A:18:ARG:HD2	2:A:533:HOH:O	2.13	0.48
1:C:89:ARG:HB2	1:C:391:ILE:CG2	2.44	0.48
1:B:337:ARG:CD	2:B:514:HOH:O	2.57	0.48
1:C:315:THR:CG2	1:C:317:ALA:H	2.26	0.48
1:B:100:ALA:HB1	1:B:112:VAL:CG2	2.44	0.48
1:C:131:ARG:NH2	1:D:143:ASP:OD2	2.47	0.48
1:E:178:ARG:HD2	1:E:182:ASP:OD2	2.13	0.48
1:A:161:GLY:N	1:A:165:GLU:OE1	2.47	0.47
1:A:300:GLY:N	1:A:301:PRO:CD	2.77	0.47
1:B:242:LEU:HD12	1:B:242:LEU:O	2.15	0.47
1:F:38:GLY:HA3	1:F:206:ILE:HD12	1.96	0.47
1:B:337:ARG:NH1	1:B:337:ARG:CG	2.72	0.47
1:A:301:PRO:HD3	1:A:390:CYS:HA	1.96	0.47
1:C:323:GLU:OE1	1:C:368:ARG:NH2	2.47	0.47
1:F:18:ARG:HG3	1:F:223:GLU:HB3	1.97	0.47
1:C:15:PRO:HD3	1:C:205:ILE:HG23	1.96	0.47
1:E:358:LEU:CD1	1:E:368:ARG:HH12	2.22	0.47
1:F:354:SER:O	1:F:358:LEU:HB2	2.15	0.47
1:D:60:PRO:HD2	2:D:546:HOH:O	2.14	0.47
1:B:167:ALA:HB2	1:B:328:PHE:CD2	2.50	0.47
1:A:302:VAL:HB	1:A:303:PRO:HD2	1.97	0.46
1:C:67:ILE:O	1:C:67:ILE:HG12	2.14	0.46
1:D:326:GLU:HB3	1:D:356:ILE:HG13	1.97	0.46
1:E:55:LEU:HA	1:E:115:GLY:O	2.15	0.46
1:F:302:VAL:HB	1:F:303:PRO:CD	2.45	0.46
1:B:269:THR:HB	1:B:270:PRO:HD2	1.96	0.46
1:D:88:ARG:HG2	1:D:391:ILE:HD13	1.96	0.46
1:B:244:GLN:HG2	1:B:244:GLN:H	1.51	0.46
1:F:259:ASN:OD1	1:F:360:HIS:N	2.47	0.46
1:F:286:SER:HA	2:F:517:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:THR:HB	1:F:295:ASP:O	2.16	0.46
1:F:191:ARG:NH1	1:F:349:THR:O	2.48	0.46
1:A:245:ASP:OD1	1:A:246:PRO:HD2	2.16	0.46
1:D:120:MET:HA	1:D:123:VAL:HG23	1.97	0.46
1:F:195:ALA:HB1	1:F:200:VAL:CG2	2.45	0.46
1:C:391:ILE:CB	1:C:395:GLN:HB2	2.41	0.45
1:D:371:ALA:O	1:D:375:ARG:HG3	2.16	0.45
1:C:86:VAL:HG12	1:D:86:VAL:HG12	1.98	0.45
1:E:99:GLN:NE2	1:E:103:GLN:OE1	2.42	0.45
1:A:403:ARG:HD2	2:A:513:HOH:O	2.16	0.45
1:B:255:SER:HB3	1:B:328:PHE:CD1	2.49	0.45
1:C:7:VAL:HG22	1:C:268:THR:O	2.16	0.45
1:E:61:ASN:OD1	1:E:63:GLU:HB2	2.16	0.45
1:F:319:ILE:O	1:F:348:ARG:NH1	2.50	0.45
1:E:184:LEU:CD1	1:E:184:LEU:C	2.85	0.45
1:F:171:ARG:HD2	1:F:249:THR:OG1	2.17	0.45
1:A:373:LEU:O	1:A:377:LEU:HB2	2.17	0.45
1:A:171:ARG:HD2	1:A:172:ARG:CA	2.47	0.45
1:E:10:GLU:N	1:E:11:PRO:HD3	2.32	0.45
1:A:45:ILE:CD1	1:A:276:LEU:HB3	2.45	0.44
1:C:255:SER:CB	1:C:328:PHE:HD1	2.28	0.44
1:E:45:ILE:HD11	1:E:276:LEU:HB3	1.99	0.44
1:E:45:ILE:CD1	1:E:276:LEU:HB3	2.47	0.44
1:A:18:ARG:HG3	1:A:223:GLU:HB3	1.99	0.44
1:A:326:GLU:HB3	1:A:356:ILE:CD1	2.47	0.44
1:D:405:GLN:HA	1:D:405:GLN:HE21	1.81	0.44
1:D:131:ARG:HG2	1:D:132:TRP:CD1	2.52	0.44
1:E:169:ASN:OD1	1:E:172:ARG:NH2	2.51	0.44
1:E:293:ALA:HA	1:E:294:PRO:HD3	1.89	0.44
1:F:279:LYS:HE2	1:F:378:HIS:CE1	2.53	0.44
1:A:255:SER:CB	1:A:328:PHE:HD1	2.31	0.44
1:B:67:ILE:HG22	1:B:85:GLN:HB2	2.00	0.44
1:F:298:GLY:O	1:F:331:GLN:NE2	2.30	0.44
1:F:59:TYR:N	1:F:60:PRO:CD	2.81	0.44
1:B:101:CYS:O	1:B:105:ARG:HG3	2.18	0.43
1:B:79:ILE:H	1:B:79:ILE:HG13	1.58	0.43
1:D:300:GLY:N	1:D:301:PRO:CD	2.80	0.43
1:E:212:THR:CB	1:E:215:GLY:O	2.65	0.43
1:F:371:ALA:O	1:F:375:ARG:HG3	2.17	0.43
1:A:11:PRO:O	1:A:375:ARG:NH1	2.50	0.43
1:A:157:HIS:CD2	1:A:157:HIS:N	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD12	1:B:241:LEU:HG	2.00	0.43
1:D:242:LEU:HD12	1:D:246:PRO:HA	2.00	0.43
1:D:89:ARG:HB2	1:D:391:ILE:CG2	2.49	0.43
1:E:80:THR:O	1:E:82:PRO:HD3	2.18	0.43
1:E:57:HIS:HB3	1:E:85:GLN:CG	2.48	0.43
1:B:343:GLU:HG2	1:B:343:GLU:O	2.18	0.43
1:D:131:ARG:HG2	1:D:132:TRP:NE1	2.34	0.43
1:B:307:VAL:HG12	1:B:311:LYS:HE2	2.00	0.43
1:F:23:PHE:HB2	2:F:503:HOH:O	2.19	0.43
1:A:10:GLU:N	1:A:11:PRO:CD	2.81	0.43
1:B:300:GLY:N	1:B:301:PRO:CD	2.81	0.43
1:D:184:LEU:O	1:D:184:LEU:HG	2.19	0.43
1:D:368:ARG:HG2	1:D:368:ARG:O	2.18	0.43
1:F:272:LYS:O	1:F:276:LEU:HG	2.19	0.43
1:B:141:ILE:CG1	1:C:141:ILE:HD12	2.47	0.43
1:D:244:GLN:HG2	1:D:244:GLN:H	1.63	0.43
1:E:88:ARG:HG2	1:E:391:ILE:HD13	2.01	0.43
1:F:327:ALA:C	1:F:328:PHE:CD1	2.92	0.43
1:A:6:ALA:HB2	1:A:105:ARG:HG3	2.01	0.42
1:A:388:THR:HA	1:A:397:LEU:O	2.19	0.42
1:C:303:PRO:O	1:C:307:VAL:HG23	2.18	0.42
1:D:161:GLY:HA3	1:D:165:GLU:HB2	2.00	0.42
1:D:321:LEU:HD11	1:D:376:GLU:CG	2.49	0.42
1:F:315:THR:CG2	1:F:316:LEU:N	2.81	0.42
1:A:269:THR:OG1	1:A:271:GLU:HG2	2.19	0.42
1:C:184:LEU:HD23	1:C:329:ALA:CB	2.48	0.42
1:C:283:ARG:NH2	1:C:402:GLU:OE1	2.52	0.42
1:C:8:ILE:CD1	1:C:267:VAL:HG22	2.49	0.42
1:D:7:VAL:HG22	1:D:268:THR:O	2.19	0.42
1:E:55:LEU:HD22	1:E:68:GLY:CA	2.43	0.42
1:F:205:ILE:HD13	1:F:205:ILE:HA	1.77	0.42
1:F:328:PHE:CD1	1:F:328:PHE:N	2.85	0.42
1:A:352:ARG:HA	1:A:352:ARG:HD3	1.73	0.42
1:B:77:LEU:O	2:B:503:HOH:O	2.22	0.42
1:C:40:LEU:HD11	1:C:77:LEU:HD11	2.02	0.42
1:A:123:VAL:O	1:B:131:ARG:NH1	2.53	0.42
1:E:397:LEU:HA	1:E:397:LEU:HD12	1.84	0.42
1:E:53:VAL:HG12	1:E:55:LEU:HD13	2.00	0.42
1:A:387:GLU:O	1:A:398:ALA:HA	2.19	0.42
1:E:56:GLY:O	1:E:116:GLY:HA2	2.19	0.42
1:A:255:SER:HB2	1:A:328:PHE:HD1	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLU:HB3	1:A:356:ILE:HD12	2.02	0.42
1:D:271:GLU:CD	1:D:271:GLU:N	2.73	0.42
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.90	0.42
1:B:299:ILE:HD12	1:B:299:ILE:HA	1.95	0.42
1:E:300:GLY:N	1:E:301:PRO:HD2	2.35	0.42
1:C:105:ARG:HB3	1:C:105:ARG:HE	1.80	0.42
1:D:239:PRO:HA	1:D:251:THR:HG22	2.01	0.42
1:D:302:VAL:HB	1:D:303:PRO:CD	2.50	0.42
1:E:201:LEU:HA	1:E:201:LEU:HD12	1.76	0.42
1:E:244:GLN:HG2	1:E:244:GLN:H	1.58	0.42
1:B:256:SER:HB3	1:B:355:GLY:O	2.20	0.41
1:D:55:LEU:HA	1:D:115:GLY:O	2.19	0.41
1:C:201:LEU:HA	1:C:201:LEU:HD12	1.80	0.41
1:D:140:GLN:HA	2:D:551:HOH:O	2.20	0.41
1:D:45:ILE:HA	1:D:45:ILE:HD12	1.90	0.41
1:A:127:SER:OG	1:A:140:GLN:O	2.10	0.41
1:C:259:ASN:OD1	1:C:359:GLY:CA	2.68	0.41
1:C:59:TYR:N	1:C:60:PRO:CD	2.83	0.41
1:D:55:LEU:CD2	1:D:68:GLY:HA2	2.44	0.41
1:E:65:PRO:HB3	1:F:89:ARG:CZ	2.50	0.41
1:B:4:ARG:NH2	1:B:107:GLY:HA2	2.36	0.41
1:B:287:TRP:O	1:B:311:LYS:CE	2.66	0.41
1:B:89:ARG:HB2	1:B:391:ILE:CG2	2.50	0.41
1:C:352:ARG:HA	1:C:352:ARG:HD3	1.82	0.41
1:D:58:CYS:C	1:D:60:PRO:HD3	2.40	0.41
1:F:174:TYR:OH	1:F:338:GLU:OE2	2.25	0.41
1:B:358:LEU:HD13	1:B:368:ARG:HD2	2.02	0.41
1:C:45:ILE:HD11	1:C:276:LEU:CD1	2.44	0.41
1:A:151:THR:OG1	1:B:62:SER:O	2.29	0.41
1:D:397:LEU:HD12	1:D:397:LEU:HA	1.86	0.41
1:E:403:ARG:HD2	2:E:521:HOH:O	2.20	0.41
1:F:287:TRP:O	1:F:311:LYS:HE3	2.20	0.41
1:D:343:GLU:O	1:D:346:HIS:HB2	2.21	0.41
1:E:57:HIS:HB3	1:E:85:GLN:HG2	2.02	0.41
1:B:45:ILE:HD13	1:B:45:ILE:HA	1.88	0.41
1:C:43:THR:HG22	2:C:542:HOH:O	2.20	0.41
1:D:178:ARG:NH2	1:D:239:PRO:HG3	2.36	0.41
1:F:6:ALA:HB2	1:F:105:ARG:HG3	2.03	0.41
1:B:300:GLY:N	1:B:301:PRO:HD2	2.36	0.41
1:B:364:ALA:HA	2:B:542:HOH:O	2.21	0.41
1:C:309:LEU:HD11	1:C:316:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ARG:O	1:F:381:GLU:HB2	2.21	0.41
1:A:59:TYR:N	1:A:60:PRO:CD	2.84	0.41
1:C:8:ILE:HD12	1:C:267:VAL:HG22	2.03	0.41
1:D:125:PHE:CZ	1:D:143:ASP:HB2	2.56	0.41
1:C:90:CYS:HA	1:C:362:VAL:CG1	2.51	0.40
1:A:184:LEU:CA	1:A:187:ARG:NH1	2.79	0.40
1:F:79:ILE:HG13	1:F:79:ILE:H	1.73	0.40
1:F:307:VAL:O	1:F:311:LYS:HG3	2.21	0.40
1:B:171:ARG:C	1:B:171:ARG:HD2	2.42	0.40
1:C:185:ALA:O	1:C:189:HIS:HD2	2.05	0.40
1:C:45:ILE:HA	1:C:45:ILE:HD13	1.69	0.40
1:D:156:PHE:HA	1:E:275:GLU:O	2.22	0.40
1:E:283:ARG:NH2	1:E:402:GLU:OE1	2.55	0.40
1:F:111:LEU:O	1:F:112:VAL:CG1	2.69	0.40
1:F:161:GLY:N	1:F:165:GLU:OE1	2.53	0.40
1:F:245:ASP:HA	1:F:246:PRO:HD3	1.92	0.40
1:A:299:ILE:O	1:A:303:PRO:HD2	2.21	0.40
1:A:394:GLY:O	1:B:69:ARG:NH2	2.55	0.40
1:F:66:ALA:O	1:F:68:GLY:N	2.54	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	393/413 (95%)	388 (99%)	5 (1%)	0	100	100
1	B	396/413 (96%)	391 (99%)	5 (1%)	0	100	100
1	C	391/413 (95%)	385 (98%)	6 (2%)	0	100	100
1	D	395/413 (96%)	393 (100%)	2 (0%)	0	100	100
1	E	394/413 (95%)	392 (100%)	2 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	383/413 (93%)	380 (99%)	3 (1%)	0	100	100
All	All	2352/2478 (95%)	2329 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	282/315 (90%)	253 (90%)	29 (10%)	9	10
1	B	302/315 (96%)	272 (90%)	30 (10%)	10	10
1	C	290/315 (92%)	265 (91%)	25 (9%)	13	16
1	D	298/315 (95%)	276 (93%)	22 (7%)	17	22
1	E	296/315 (94%)	271 (92%)	25 (8%)	14	17
1	F	281/315 (89%)	249 (89%)	32 (11%)	7	7
All	All	1749/1890 (92%)	1586 (91%)	163 (9%)	11	13

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	26	LEU
1	A	37	LYS
1	A	45	ILE
1	A	79	ILE
1	A	157	HIS
1	A	171	ARG
1	A	177	SER
1	A	178	ARG
1	A	187	ARG
1	A	198	GLU
1	A	201	LEU
1	A	210	VAL

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Mol	Chain	Res	Type
1	A	226	ARG
1	A	244	GLN
1	A	251	THR
1	A	256	SER
1	A	297	MET
1	A	311	LYS
1	A	315	THR
1	A	316	LEU
1	A	325	ASN
1	A	341	PHE
1	A	348	ARG
1	A	354	SER
1	A	373	LEU
1	A	377	LEU
1	A	383	ARG
1	A	389	MET
1	B	37	LYS
1	B	55	LEU
1	B	89	ARG
1	B	131	ARG
1	B	155	LYS
1	B	164	LEU
1	B	171	ARG
1	B	175[A]	HIS
1	B	175[B]	HIS
1	B	178	ARG
1	B	180	GLU
1	B	197[A]	SER
1	B	197[B]	SER
1	B	201	LEU
1	B	216	GLU
1	B	226	ARG
1	B	229	THR
1	B	238	LYS
1	B	244	GLN
1	B	249	THR
1	B	255	SER
1	B	279	LYS
1	B	297	MET
1	B	315	THR
1	B	316	LEU
1	B	337	ARG

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Mol	Chain	Res	Type
1	B	348	ARG
1	B	352	ARG
1	B	373	LEU
1	B	377	LEU
1	C	4	ARG
1	C	22	MET
1	C	26	LEU
1	C	55	LEU
1	C	79	ILE
1	C	103	GLN
1	C	105	ARG
1	C	127	SER
1	C	136	ARG
1	C	176	ILE
1	C	178	ARG
1	C	188	SER
1	C	201	LEU
1	C	216	GLU
1	C	217	GLU
1	C	220	SER
1	C	297	MET
1	C	315	THR
1	C	316	LEU
1	C	340	LYS
1	C	341	PHE
1	C	347	GLU
1	C	373	LEU
1	C	377	LEU
1	C	389	MET
1	D	26	LEU
1	D	45	ILE
1	D	55	LEU
1	D	79	ILE
1	D	89	ARG
1	D	150	THR
1	D	180	GLU
1	D	201	LEU
1	D	210	VAL
1	D	217	GLU
1	D	228	ASP
1	D	256	SER
1	D	279	LYS

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Mol	Chain	Res	Type
1	D	297	MET
1	D	315	THR
1	D	316	LEU
1	D	352	ARG
1	D	368	ARG
1	D	373	LEU
1	D	377	LEU
1	D	405	GLN
1	D	406	GLU
1	E	55	LEU
1	E	89	ARG
1	E	131	ARG
1	E	137	THR
1	E	164	LEU
1	E	178	ARG
1	E	184	LEU
1	E	201	LEU
1	E	220	SER
1	E	243	LYS
1	E	244	GLN
1	E	256	SER
1	E	263	SER
1	E	297	MET
1	E	314	LEU
1	E	315	THR
1	E	316	LEU
1	E	324	LEU
1	E	328	PHE
1	E	347	GLU
1	E	354	SER
1	E	368	ARG
1	E	373	LEU
1	E	377	LEU
1	E	405	GLN
1	F	4	ARG
1	F	24	ARG
1	F	45	ILE
1	F	55	LEU
1	F	89	ARG
1	F	155	LYS
1	F	164	LEU
1	F	166	THR

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Mol	Chain	Res	Type
1	F	171	ARG
1	F	176	ILE
1	F	178	ARG
1	F	183	GLU
1	F	197	SER
1	F	201	LEU
1	F	229	THR
1	F	234	LEU
1	F	241	LEU
1	F	247	GLU
1	F	249	THR
1	F	272	LYS
1	F	283	ARG
1	F	297	MET
1	F	299	ILE
1	F	314	LEU
1	F	316	LEU
1	F	324	LEU
1	F	340	LYS
1	F	373	LEU
1	F	377	LEU
1	F	379	ARG
1	F	383	ARG
1	F	389	MET

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

Mol	Chain	Res	Type
1	A	157	HIS
1	A	244	GLN
1	C	189	HIS
1	D	157	HIS
1	D	405	GLN

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 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	399/413 (96%)	0.05	12 (3%) 54 57	17, 37, 69, 89	0
1	B	398/413 (96%)	-0.21	0 100 100	16, 31, 52, 75	0
1	C	397/413 (96%)	-0.01	3 (0%) 87 89	17, 38, 67, 84	0
1	D	398/413 (96%)	-0.23	1 (0%) 94 95	17, 32, 51, 74	0
1	E	400/413 (96%)	-0.00	3 (0%) 87 89	22, 36, 61, 78	0
1	F	393/413 (95%)	0.34	19 (4%) 34 37	24, 43, 68, 84	0
All	All	2385/2478 (96%)	-0.01	38 (1%) 74 77	16, 36, 65, 89	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ALA	4.0
1	C	240	VAL	3.7
1	A	229	THR	3.6
1	E	214	ASP	3.3
1	F	334	ALA	3.2
1	F	184	LEU	3.0
1	E	215	GLY	2.8
1	A	228	ASP	2.8
1	F	384	TYR	2.8
1	F	181	GLN	2.7
1	F	234	LEU	2.7
1	A	246	PRO	2.7
1	F	156	PHE	2.7
1	A	214	ASP	2.7
1	F	194	ALA	2.7
1	A	313	GLY	2.6
1	F	221	VAL	2.5
1	F	229	THR	2.4
1	F	230	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	237	LEU	2.4
1	E	212	THR	2.4
1	F	98	ILE	2.3
1	C	174	TYR	2.3
1	F	330	ALA	2.3
1	F	240	VAL	2.2
1	A	235	ALA	2.2
1	A	244	GLN	2.2
1	F	295	ASP	2.2
1	F	328	PHE	2.2
1	A	234	LEU	2.2
1	F	227	ALA	2.2
1	F	313	GLY	2.2
1	F	377	LEU	2.2
1	A	226	ARG	2.1
1	A	212	THR	2.1
1	D	210	VAL	2.1
1	A	233	ALA	2.0
1	C	246	PRO	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.