



# Full wwPDB X-ray Structure Validation Report i

May 14, 2020 – 03:48 pm BST

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](mailto: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 i symbol.

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The following versions of software and data (see references ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11



## 2 Entry composition [\(i\)](#)

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

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





- Molecule 1: Beta-ketothiolase

Chain D: 



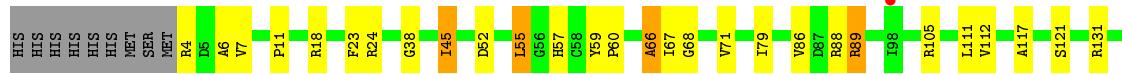
- Molecule 1: Beta-ketothiolase

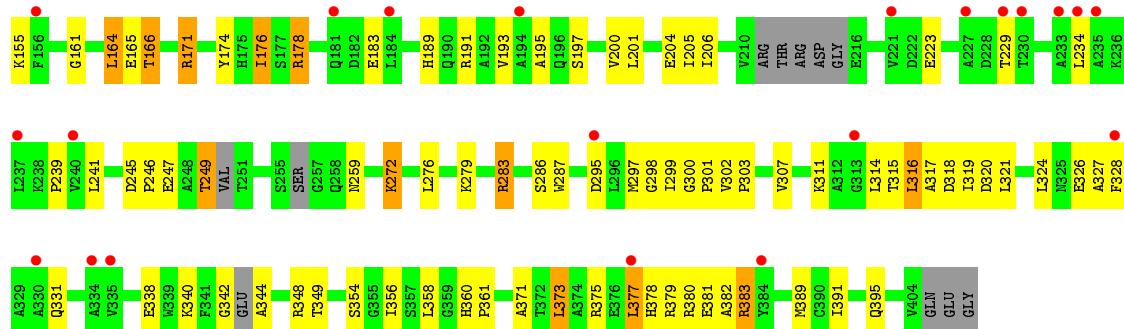
Chain E: 



- Molecule 1: Beta-ketothiolase

Chain F: 





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.46 Å    181.47 Å    271.73 Å 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
$< I/\sigma(I) >$ <sup>1</sup>	1.72 (at 2.45 Å)	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 (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.9	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.





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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 [\(i\)](#)

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	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: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:332:ALA:O	1:D:336:MET:HG3	2.05	0.56
1:D:11:PRO:O	1:D:375:ARG:NH1	2.39	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:166:THR:HG22	1:C:295:ASP:O	2.12	0.49

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<b>Atom-1</b>	<b>Atom-2</b>	<b>Interatomic distance (Å)</b>	<b>Clash overlap (Å)</b>
1:F:286:SER:HA	2:F:517:HOH:O	2.14	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:157:HIS:CD2	1:A:157:HIS:N	2.85	0.43
1:A:11:PRO:O	1:A:375:ARG:NH1	2.50	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:57:HIS:HB3	1:E:85:GLN:CG	2.48	0.43
1:E:80:THR:O	1:E:82:PRO:HD3	2.18	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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	282/315 (90%)	253 (90%)	29 (10%)	7 7
1	B	302/315 (96%)	272 (90%)	30 (10%)	8 7
1	C	290/315 (92%)	265 (91%)	25 (9%)	10 11
1	D	298/315 (95%)	276 (93%)	22 (7%)	13 16
1	E	296/315 (94%)	271 (92%)	25 (8%)	11 12
1	F	281/315 (89%)	249 (89%)	32 (11%)	5 5
All	All	1749/1890 (92%)	1586 (91%)	163 (9%)	9 9

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 [\(i\)](#)

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.



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Mol	Chain	Res	Type	RSRZ
1	F	221	VAL	2.5
1	A	214	ASP	2.5
1	F	229	THR	2.4
1	F	330	ALA	2.4
1	F	240	VAL	2.3
1	F	377	LEU	2.3
1	F	98	ILE	2.2
1	F	295	ASP	2.2
1	A	235	ALA	2.2
1	A	244	GLN	2.2
1	F	227	ALA	2.2
1	A	226	ARG	2.1
1	F	313	GLY	2.1
1	F	328	PHE	2.1
1	A	234	LEU	2.1
1	F	335	VAL	2.1
1	F	235	ALA	2.1
1	C	246	PRO	2.0
1	F	233	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.