



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 04:16 AM EDT

PDB ID : 3G7K / pdb_00003g7k
Title : Crystal Structure of Methylitaconate-delta-isomerase
Authors : Messerschmidt, A.; Macieira, S.; Velarde, M.
Deposited on : 2009-02-10
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

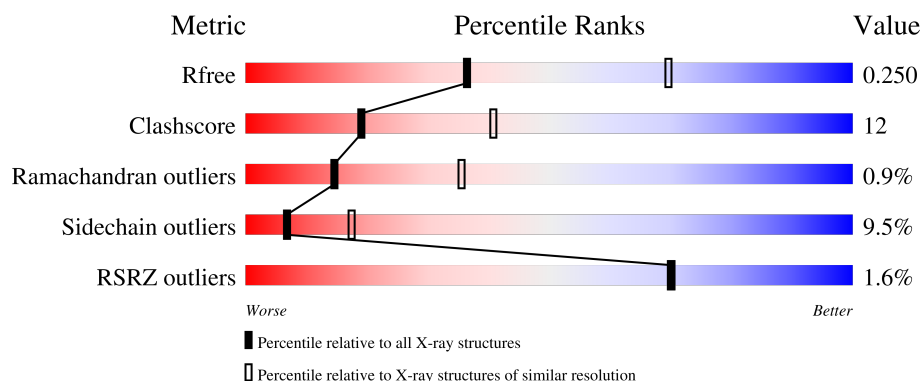
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	391	 77% 16% . .
1	B	391	 74% 21% . .
1	C	391	 39% 14% . 43%
1	D	391	 74% 20% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10592 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 3-methylitaconate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2807	1757	474	558	18			
1	B	387	Total	C	N	O	S	0	0	0
			2868	1795	486	569	18			
1	C	224	Total	C	N	O	S	0	0	0
			1645	1033	284	319	9			
1	D	379	Total	C	N	O	S	0	0	0
			2807	1757	474	558	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	GLY	-	expression tag	UNP Q0QLE6
A	382	SER	-	expression tag	UNP Q0QLE6
A	383	ALA	-	expression tag	UNP Q0QLE6
A	384	TRP	-	expression tag	UNP Q0QLE6
A	385	SER	-	expression tag	UNP Q0QLE6
A	386	HIS	-	expression tag	UNP Q0QLE6
A	387	PRO	-	expression tag	UNP Q0QLE6
A	388	GLN	-	expression tag	UNP Q0QLE6
A	389	PHE	-	expression tag	UNP Q0QLE6
A	390	GLU	-	expression tag	UNP Q0QLE6
A	391	LYS	-	expression tag	UNP Q0QLE6
B	381	GLY	-	expression tag	UNP Q0QLE6
B	382	SER	-	expression tag	UNP Q0QLE6
B	383	ALA	-	expression tag	UNP Q0QLE6
B	384	TRP	-	expression tag	UNP Q0QLE6
B	385	SER	-	expression tag	UNP Q0QLE6
B	386	HIS	-	expression tag	UNP Q0QLE6
B	387	PRO	-	expression tag	UNP Q0QLE6
B	388	GLN	-	expression tag	UNP Q0QLE6
B	389	PHE	-	expression tag	UNP Q0QLE6
B	390	GLU	-	expression tag	UNP Q0QLE6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	391	LYS	-	expression tag	UNP Q0QLE6
C	381	GLY	-	expression tag	UNP Q0QLE6
C	382	SER	-	expression tag	UNP Q0QLE6
C	383	ALA	-	expression tag	UNP Q0QLE6
C	384	TRP	-	expression tag	UNP Q0QLE6
C	385	SER	-	expression tag	UNP Q0QLE6
C	386	HIS	-	expression tag	UNP Q0QLE6
C	387	PRO	-	expression tag	UNP Q0QLE6
C	388	GLN	-	expression tag	UNP Q0QLE6
C	389	PHE	-	expression tag	UNP Q0QLE6
C	390	GLU	-	expression tag	UNP Q0QLE6
C	391	LYS	-	expression tag	UNP Q0QLE6
D	381	GLY	-	expression tag	UNP Q0QLE6
D	382	SER	-	expression tag	UNP Q0QLE6
D	383	ALA	-	expression tag	UNP Q0QLE6
D	384	TRP	-	expression tag	UNP Q0QLE6
D	385	SER	-	expression tag	UNP Q0QLE6
D	386	HIS	-	expression tag	UNP Q0QLE6
D	387	PRO	-	expression tag	UNP Q0QLE6
D	388	GLN	-	expression tag	UNP Q0QLE6
D	389	PHE	-	expression tag	UNP Q0QLE6
D	390	GLU	-	expression tag	UNP Q0QLE6
D	391	LYS	-	expression tag	UNP Q0QLE6

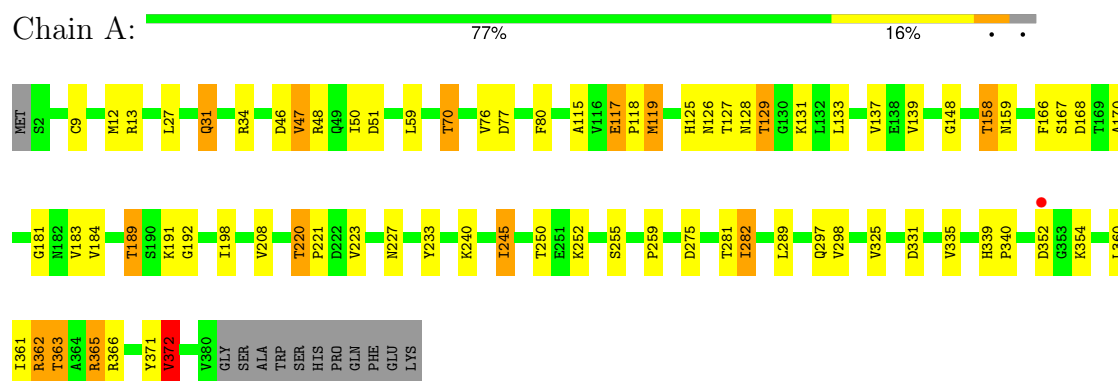
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	129	Total O 129 129	0	0
2	B	107	Total O 107 107	0	0
2	C	77	Total O 77 77	0	0
2	D	152	Total O 152 152	0	0

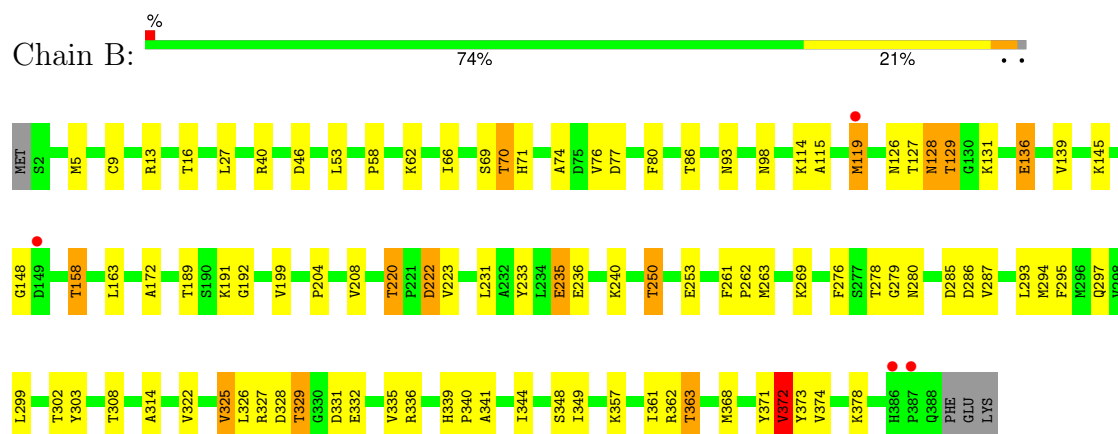
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

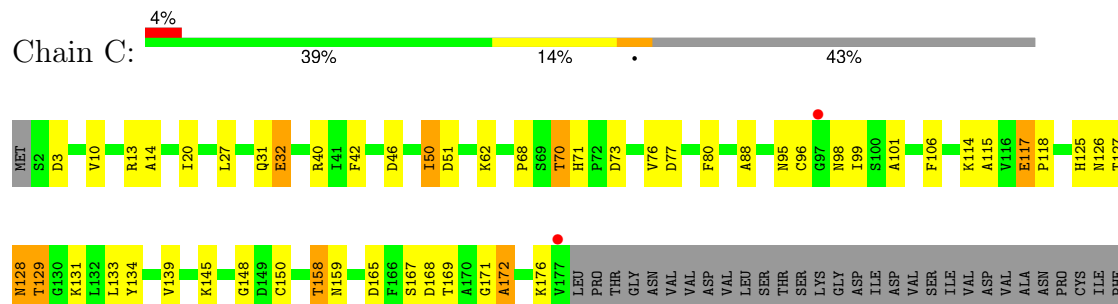
• Molecule 1: 3-methylitaconate isomerase

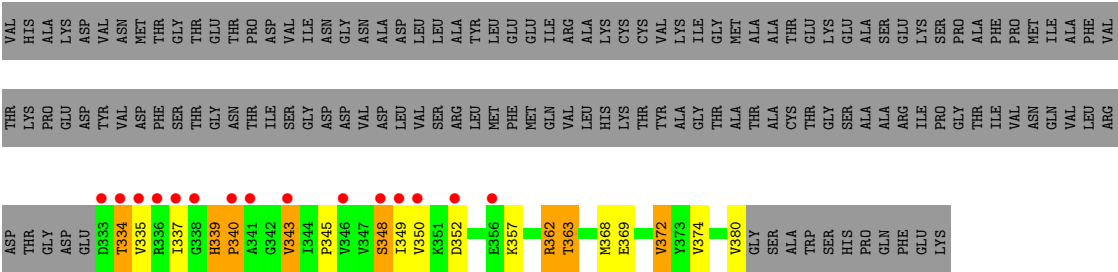


• Molecule 1: 3-methylitaconate isomerase

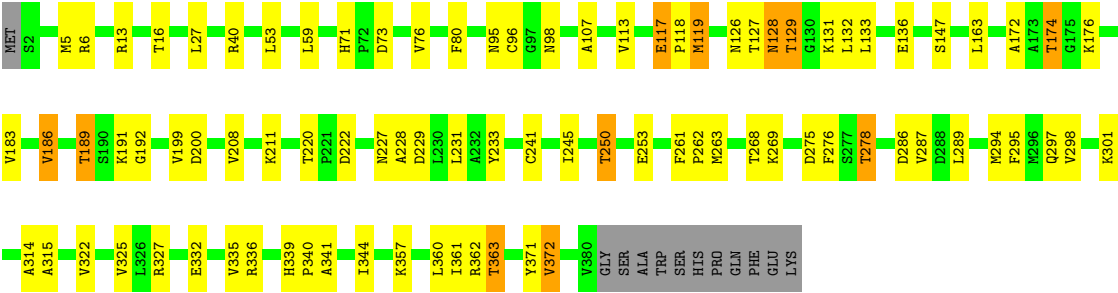


• Molecule 1: 3-methylitaconate isomerase





● Molecule 1: 3-methylitaconate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.08Å 142.08Å 228.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.70) 97.7 (50.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.256 0.199 , 0.250	Depositor DCC
R_{free} test set	2402 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10592	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 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	0/2849	1.06	9/3871 (0.2%)
1	B	0.73	0/2914	0.97	4/3961 (0.1%)
1	C	0.79	1/1669 (0.1%)	1.05	6/2265 (0.3%)
1	D	0.81	1/2849 (0.0%)	1.03	2/3871 (0.1%)
All	All	0.78	2/10281 (0.0%)	1.03	21/13968 (0.2%)

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	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	350	VAL	CA-CB	6.60	1.60	1.53
1	D	186	VAL	CA-CB	5.09	1.60	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	GLU	CA-C-N	16.29	140.20	119.84
1	A	117	GLU	C-N-CA	16.29	140.20	119.84
1	D	117	GLU	CA-C-N	15.81	139.61	119.84
1	D	117	GLU	C-N-CA	15.81	139.61	119.84
1	C	117	GLU	CA-C-N	10.09	132.46	119.84
1	C	117	GLU	C-N-CA	10.09	132.46	119.84
1	A	372	VAL	CB-CA-C	-7.50	101.28	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	VAL	CB-CA-C	-5.82	103.60	111.63
1	C	76	VAL	N-CA-C	5.80	115.48	108.06
1	A	181	GLY	N-CA-C	-5.43	108.22	114.69
1	A	167	SER	N-CA-C	5.40	117.25	111.36
1	B	127	THR	N-CA-C	5.39	116.84	111.07
1	A	70	THR	N-CA-C	-5.29	105.13	113.02
1	B	71	HIS	CA-C-N	5.29	126.45	119.84
1	B	71	HIS	C-N-CA	5.29	126.45	119.84
1	A	354	LYS	N-CA-C	5.26	118.13	109.72
1	C	339	HIS	CA-C-N	5.23	126.38	119.84
1	C	339	HIS	C-N-CA	5.23	126.38	119.84
1	A	159	ASN	N-CA-C	5.17	116.15	108.86
1	A	227	ASN	N-CA-C	5.15	117.03	108.02
1	B	372	VAL	CB-CA-C	-5.11	104.08	111.34

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	GLU	Peptide
1	C	117	GLU	Peptide
1	D	117	GLU	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	2807	0	2819	55	0
1	B	2868	0	2869	80	0
1	C	1645	0	1652	46	0
1	D	2807	0	2819	66	0
2	A	129	0	0	5	0
2	B	107	0	0	5	0
2	C	77	0	0	5	0
2	D	152	0	0	8	0
All	All	10592	0	10159	236	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 12.

All (236) 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:D:13:ARG:NH2	1:D:363:THR:HG22	1.45	1.31
1:D:297:GLN:HG3	2:D:434:HOH:O	1.34	1.28
1:A:13:ARG:NH2	1:A:363:THR:HG22	1.51	1.25
1:B:13:ARG:NH2	1:B:363:THR:HG22	1.53	1.21
1:D:13:ARG:HH22	1:D:363:THR:CG2	1.56	1.18
1:A:13:ARG:HH22	1:A:363:THR:CG2	1.60	1.12
1:C:13:ARG:NH2	1:C:363:THR:HG23	1.66	1.10
1:C:13:ARG:HH21	1:C:363:THR:HG23	1.09	1.08
1:B:13:ARG:HH22	1:B:363:THR:CG2	1.68	1.06
1:D:13:ARG:HH22	1:D:363:THR:HG22	0.92	1.04
1:D:96:CYS:SG	2:D:448:HOH:O	2.14	1.04
1:B:13:ARG:HH22	1:B:363:THR:HG22	1.03	1.03
1:B:287:VAL:O	1:B:327:ARG:NH1	1.96	0.97
1:A:189:THR:HG22	1:A:191:LYS:H	1.28	0.97
1:D:95:ASN:ND2	1:D:96:CYS:H	1.62	0.96
1:B:189:THR:HG22	1:B:191:LYS:H	1.30	0.95
1:D:95:ASN:HD22	1:D:96:CYS:H	1.12	0.94
1:B:126:ASN:ND2	1:B:129:THR:HB	1.86	0.91
1:B:126:ASN:HD22	1:B:129:THR:HB	1.37	0.88
1:D:126:ASN:HD22	1:D:129:THR:HB	1.39	0.88
1:B:80:PHE:H	1:B:128:ASN:HD21	1.14	0.87
1:C:71:HIS:HD2	1:C:73:ASP:H	1.20	0.87
1:C:148:GLY:O	1:C:158:THR:HG23	1.72	0.86
1:D:71:HIS:HD2	1:D:73:ASP:H	1.22	0.86
1:A:148:GLY:O	1:A:158:THR:HG23	1.76	0.85
1:A:80:PHE:H	1:A:128:ASN:HD21	1.19	0.85
1:B:189:THR:HB	1:B:192:GLY:O	1.77	0.84
1:D:80:PHE:H	1:D:128:ASN:HD21	1.26	0.83
1:C:126:ASN:HD22	1:C:129:THR:HB	1.43	0.83
1:D:250:THR:HG22	1:D:253:GLU:H	1.46	0.81
1:D:129:THR:HG22	1:D:131:LYS:H	1.47	0.80
1:B:250:THR:HG22	1:B:253:GLU:H	1.48	0.79
1:D:363:THR:HG21	2:D:408:HOH:O	1.83	0.79
1:B:129:THR:HG21	2:B:477:HOH:O	1.85	0.77
1:D:126:ASN:ND2	1:D:129:THR:HB	2.00	0.77
1:D:189:THR:CG2	1:D:191:LYS:H	1.97	0.77
1:C:129:THR:HG22	1:C:131:LYS:H	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ASN:HD22	1:D:96:CYS:N	1.83	0.76
1:C:334:THR:HG22	1:C:345:PRO:HB2	1.70	0.74
1:B:371:TYR:OH	1:C:369:GLU:OE2	2.06	0.73
1:D:174:THR:HG22	1:D:176:LYS:H	1.53	0.73
1:B:278:THR:O	1:B:280:ASN:N	2.18	0.72
1:D:189:THR:HG22	1:D:191:LYS:H	1.55	0.71
1:B:189:THR:HG22	1:B:191:LYS:N	2.06	0.70
1:B:40:ARG:NH2	1:B:378:LYS:HD2	2.07	0.69
1:A:275:ASP:HB2	1:A:282:ILE:CD1	2.24	0.67
1:A:363:THR:HG21	2:A:451:HOH:O	1.93	0.67
1:A:189:THR:HB	1:A:192:GLY:O	1.94	0.67
1:B:189:THR:HG21	1:B:233:TYR:CE1	2.30	0.66
1:B:189:THR:CG2	1:B:233:TYR:HE1	2.09	0.66
1:B:129:THR:HG22	1:B:131:LYS:H	1.61	0.65
1:D:95:ASN:ND2	1:D:96:CYS:N	2.40	0.65
1:D:119:MET:HE1	1:D:136:GLU:HA	1.79	0.65
1:A:360:LEU:HD12	1:A:362:ARG:HD3	1.77	0.65
1:B:278:THR:C	1:B:280:ASN:H	2.05	0.65
1:A:129:THR:HG23	1:A:131:LYS:HG2	1.80	0.64
1:B:339:HIS:HB2	1:B:340:PRO:CD	2.28	0.63
1:C:134:TYR:HB2	1:C:165:ASP:HB3	1.79	0.63
1:B:357:LYS:HE2	2:B:462:HOH:O	1.98	0.63
1:B:331:ASP:HA	2:B:441:HOH:O	1.98	0.63
1:A:352:ASP:HA	2:A:514:HOH:O	1.97	0.62
1:B:189:THR:HG21	1:B:233:TYR:OH	1.99	0.62
1:D:13:ARG:NH2	1:D:363:THR:CG2	2.30	0.62
1:B:329:THR:HG22	1:B:332:GLU:HB3	1.81	0.62
1:C:80:PHE:H	1:C:128:ASN:HD21	1.46	0.62
1:B:53:LEU:HD11	1:B:372:VAL:HG13	1.82	0.62
1:B:220:THR:HG22	1:B:222:ASP:H	1.63	0.62
1:A:13:ARG:HH22	1:A:363:THR:HG22	0.66	0.61
1:A:339:HIS:HB2	1:A:340:PRO:CD	2.30	0.61
1:C:50:ILE:O	1:D:13:ARG:HG3	2.01	0.61
1:B:263:MET:HE3	1:B:295:PHE:HD1	1.66	0.60
1:C:168:ASP:HB3	2:C:467:HOH:O	2.01	0.60
1:C:169:THR:HG22	2:C:465:HOH:O	2.02	0.60
1:D:53:LEU:HD11	1:D:372:VAL:HG13	1.83	0.59
1:A:189:THR:CG2	1:A:191:LYS:H	2.11	0.59
1:D:189:THR:HG22	1:D:191:LYS:N	2.17	0.59
1:A:168:ASP:OD1	1:A:168:ASP:O	2.19	0.59
1:D:136:GLU:HB2	1:D:163:LEU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ILE:O	1:A:362:ARG:HD2	2.03	0.59
1:C:115:ALA:HB1	1:C:139:VAL:HG11	1.84	0.59
1:D:189:THR:HB	1:D:192:GLY:O	2.03	0.58
1:A:275:ASP:HB2	1:A:282:ILE:HD13	1.85	0.58
1:B:339:HIS:HB2	1:B:340:PRO:HD3	1.84	0.58
1:A:189:THR:HG22	1:A:191:LYS:N	2.10	0.58
1:D:16:THR:OG1	1:D:98:ASN:ND2	2.37	0.58
1:C:363:THR:HG21	2:C:407:HOH:O	2.03	0.57
1:B:363:THR:HG21	2:B:396:HOH:O	2.04	0.57
1:B:13:ARG:NH2	1:B:363:THR:CG2	2.40	0.57
1:A:50:ILE:O	1:B:13:ARG:HG3	2.04	0.57
1:D:231:LEU:HD22	1:D:294:MET:HE1	1.87	0.56
1:B:263:MET:HE3	1:B:295:PHE:CD1	2.40	0.56
1:D:189:THR:HG23	1:D:191:LYS:H	1.71	0.56
1:D:189:THR:HG21	1:D:233:TYR:OH	2.05	0.56
1:B:148:GLY:O	1:B:158:THR:HG23	2.06	0.56
1:D:339:HIS:HB2	1:D:340:PRO:CD	2.36	0.56
1:C:339:HIS:HB2	1:C:340:PRO:HD2	1.87	0.55
1:C:126:ASN:ND2	1:C:129:THR:HB	2.18	0.55
1:B:231:LEU:HD22	1:B:294:MET:HE1	1.88	0.55
1:C:128:ASN:ND2	1:C:128:ASN:H	2.05	0.55
1:B:189:THR:CG2	1:B:233:TYR:CE1	2.88	0.54
1:D:332:GLU:HG2	2:D:470:HOH:O	2.08	0.54
1:B:129:THR:HG23	1:B:131:LYS:HG2	1.89	0.53
1:D:263:MET:HE3	1:D:295:PHE:CD1	2.42	0.53
1:D:119:MET:HE1	1:D:136:GLU:CA	2.37	0.53
1:A:189:THR:HG21	1:A:233:TYR:OH	2.07	0.53
1:A:126:ASN:ND2	1:A:129:THR:HB	2.24	0.53
1:A:189:THR:CG2	1:A:233:TYR:HE1	2.21	0.53
1:C:32:GLU:HG2	2:C:464:HOH:O	2.09	0.53
1:B:269:LYS:N	1:B:325:VAL:HG22	2.24	0.53
1:A:129:THR:HG22	1:A:131:LYS:H	1.73	0.53
1:B:172:ALA:HB3	2:B:455:HOH:O	2.08	0.53
1:B:199:VAL:HG21	1:B:314:ALA:HB2	1.91	0.53
1:A:250:THR:HG22	1:A:252:LYS:H	1.72	0.52
1:D:287:VAL:O	1:D:327:ARG:NH1	2.42	0.52
1:D:339:HIS:HB2	1:D:340:PRO:HD2	1.90	0.52
1:B:327:ARG:HG2	1:B:328:ASP:O	2.10	0.52
1:C:129:THR:HG22	1:C:131:LYS:N	2.22	0.52
1:D:129:THR:CG2	1:D:131:LYS:HG2	2.39	0.52
1:B:70:THR:HB	1:B:77:ASP:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:HG23	1:A:184:VAL:HG23	1.92	0.52
1:B:204:PRO:HB2	1:B:262:PRO:HB3	1.91	0.52
1:D:276:PHE:HE1	1:D:341:ALA:HB2	1.74	0.52
1:C:369:GLU:OE2	1:D:6:ARG:NH1	2.44	0.51
1:B:189:THR:HG23	1:B:233:TYR:HE1	1.74	0.51
1:B:80:PHE:H	1:B:128:ASN:ND2	1.95	0.51
1:A:361:ILE:O	1:A:362:ARG:CD	2.59	0.51
1:B:115:ALA:HB1	1:B:139:VAL:HG11	1.92	0.51
1:B:119:MET:HE1	1:B:136:GLU:HG2	1.93	0.51
1:C:13:ARG:NH2	1:C:363:THR:CG2	2.57	0.51
1:A:12:MET:HG2	1:A:366:ARG:HA	1.93	0.51
1:D:128:ASN:HD22	1:D:128:ASN:H	1.58	0.51
1:A:115:ALA:HB1	1:A:139:VAL:HG11	1.93	0.51
1:B:9:CYS:SG	1:B:372:VAL:HG22	2.51	0.51
1:B:189:THR:HG21	1:B:233:TYR:HE1	1.73	0.51
1:C:77:ASP:OD2	1:C:125:HIS:HD2	1.94	0.51
1:C:334:THR:CG2	1:C:345:PRO:HB2	2.38	0.51
1:B:189:THR:HG21	1:B:233:TYR:CZ	2.46	0.50
1:C:171:GLY:O	1:C:172:ALA:C	2.53	0.50
1:C:96:CYS:HB3	1:C:99:ILE:HB	1.94	0.50
1:A:31:GLN:HE21	1:A:31:GLN:HA	1.77	0.50
1:D:5:MET:HE1	2:D:421:HOH:O	2.12	0.49
1:C:348:SER:O	1:C:349:ILE:HG13	2.12	0.49
1:A:31:GLN:NE2	1:A:34:ARG:HD2	2.27	0.49
1:D:276:PHE:CE1	1:D:341:ALA:HB2	2.48	0.49
1:D:53:LEU:HD11	1:D:372:VAL:CG1	2.43	0.49
1:D:71:HIS:CD2	1:D:73:ASP:H	2.14	0.49
1:A:77:ASP:OD2	1:A:125:HIS:HD2	1.95	0.49
1:D:227:ASN:C	1:D:227:ASN:HD22	2.21	0.49
1:D:129:THR:HG22	1:D:131:LYS:N	2.22	0.49
1:C:337:ILE:O	1:C:343:VAL:HA	2.13	0.48
1:A:80:PHE:H	1:A:128:ASN:ND2	2.00	0.48
1:B:236:GLU:O	1:B:240:LYS:HG3	2.14	0.48
1:C:71:HIS:CD2	1:C:73:ASP:H	2.12	0.48
1:B:9:CYS:CB	1:B:372:VAL:HG22	2.44	0.48
1:C:95:ASN:HD21	1:C:133:LEU:HD11	1.78	0.48
1:B:70:THR:CG2	1:B:70:THR:O	2.61	0.48
1:B:303:TYR:HD2	1:B:308:THR:OG1	1.97	0.48
1:B:235:GLU:HG2	1:B:297:GLN:HG3	1.96	0.47
1:B:276:PHE:HE1	1:B:341:ALA:HB2	1.80	0.47
1:A:189:THR:HG21	1:A:233:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HH22	1:D:363:THR:HG23	1.64	0.47
1:C:368:MET:HG3	1:D:371:TYR:O	2.15	0.47
1:D:199:VAL:HG21	1:D:314:ALA:HB2	1.97	0.47
1:D:107:ALA:HB1	1:D:113:VAL:HG23	1.97	0.46
1:A:245:ILE:HG23	1:A:245:ILE:O	2.16	0.46
1:A:131:LYS:NZ	1:A:170:ALA:O	2.48	0.46
1:C:98:ASN:O	1:C:101:ALA:HB3	2.16	0.46
1:C:362:ARG:HD2	1:C:362:ARG:HA	1.42	0.45
1:B:80:PHE:N	1:B:128:ASN:HD21	1.97	0.45
1:D:40:ARG:CZ	2:D:519:HOH:O	2.64	0.45
1:B:114:LYS:N	1:C:68:PRO:HG2	2.31	0.45
1:B:276:PHE:CE1	1:B:341:ALA:HB2	2.52	0.45
1:D:261:PHE:HA	1:D:262:PRO:C	2.41	0.45
1:C:80:PHE:CE1	1:C:96:CYS:HB2	2.52	0.45
1:B:69:SER:OG	1:B:74:ALA:HB3	2.17	0.44
1:B:361:ILE:O	1:B:362:ARG:HD2	2.17	0.44
1:D:361:ILE:O	1:D:362:ARG:HD2	2.17	0.44
1:C:46:ASP:OD1	1:C:46:ASP:C	2.59	0.44
1:C:70:THR:HG22	1:C:125:HIS:CD2	2.52	0.44
1:A:362:ARG:HD2	1:A:362:ARG:HA	1.60	0.44
1:B:235:GLU:OE1	1:B:235:GLU:HA	2.17	0.44
1:D:211:LYS:HD3	2:D:513:HOH:O	2.18	0.44
1:C:131:LYS:HA	1:C:131:LYS:HD3	1.73	0.44
1:A:166:PHE:CE1	1:A:360:LEU:HD21	2.53	0.44
1:C:14:ALA:HB3	1:C:99:ILE:HD13	2.00	0.44
1:C:51:ASP:OD1	1:D:13:ARG:HD3	2.18	0.44
1:A:371:TYR:O	1:B:368:MET:HG3	2.18	0.44
1:B:302:THR:O	1:B:339:HIS:HB2	2.18	0.44
1:C:20:ILE:HD12	1:C:42:PHE:CZ	2.52	0.44
1:B:349:ILE:HD12	1:B:357:LYS:HD2	2.01	0.43
1:C:150:CYS:HB3	1:C:159:ASN:O	2.19	0.43
1:A:126:ASN:HD22	1:A:129:THR:HB	1.83	0.43
1:A:129:THR:CG2	1:A:131:LYS:H	2.31	0.43
1:A:220:THR:HG22	1:A:223:VAL:H	1.83	0.43
1:B:129:THR:CG2	1:B:131:LYS:H	2.26	0.43
1:A:240:LYS:HE3	2:A:461:HOH:O	2.19	0.43
1:A:198:ILE:HG21	1:A:245:ILE:HD13	2.00	0.43
1:B:293:LEU:O	1:B:299:LEU:HD12	2.19	0.43
1:D:132:LEU:O	1:D:133:LEU:HD23	2.19	0.43
1:B:220:THR:HB	1:B:223:VAL:HG23	2.01	0.42
1:B:326:LEU:HG	1:B:327:ARG:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PHE:N	1:A:128:ASN:HD21	2.01	0.42
1:C:167:SER:HB3	1:C:357:LYS:HA	2.01	0.42
1:A:9:CYS:SG	1:A:372:VAL:HG22	2.59	0.42
1:A:119:MET:HA	1:A:137:VAL:O	2.20	0.42
1:D:275:ASP:OD1	1:D:275:ASP:C	2.62	0.42
1:D:301:LYS:HB2	1:D:301:LYS:HE2	1.82	0.42
1:B:322:VAL:O	1:B:325:VAL:HG12	2.20	0.42
1:C:3:ASP:OD2	1:D:147:SER:N	2.48	0.42
1:D:286:ASP:O	1:D:336:ARG:HD2	2.20	0.41
1:A:339:HIS:HB2	1:A:340:PRO:HD3	2.02	0.41
1:A:189:THR:HG23	1:A:233:TYR:HE1	1.84	0.41
1:A:365:ARG:NH2	1:B:373:TYR:O	2.53	0.41
1:B:126:ASN:HD22	1:B:129:THR:CB	2.20	0.41
1:D:227:ASN:O	1:D:228:ALA:C	2.62	0.41
1:A:220:THR:O	1:A:221:PRO:C	2.63	0.41
1:D:241:CYS:O	1:D:245:ILE:HG12	2.19	0.41
1:B:9:CYS:HB2	1:B:372:VAL:HG22	2.01	0.41
1:A:47:VAL:HG22	2:A:504:HOH:O	2.21	0.41
1:A:259:PRO:HB2	1:A:297:GLN:HE22	1.86	0.41
1:B:16:THR:OG1	1:B:98:ASN:ND2	2.52	0.41
1:B:128:ASN:ND2	1:B:128:ASN:H	2.18	0.41
1:C:106:PHE:CD2	1:C:106:PHE:C	2.98	0.41
1:D:129:THR:HG21	2:D:540:HOH:O	2.20	0.41
1:A:168:ASP:O	1:A:168:ASP:CG	2.64	0.41
1:B:58:PRO:O	1:B:62:LYS:HE2	2.21	0.41
1:B:286:ASP:O	1:B:336:ARG:HD2	2.21	0.41
1:C:172:ALA:HB3	2:C:458:HOH:O	2.21	0.41
1:D:278:THR:O	1:D:278:THR:CG2	2.69	0.41
1:D:174:THR:HB	1:D:200:ASP:OD2	2.22	0.40
1:D:315:ALA:HA	1:D:322:VAL:HG12	2.02	0.40
1:A:51:ASP:OD1	1:B:13:ARG:HD3	2.21	0.40
1:A:59:LEU:HD13	2:A:429:HOH:O	2.21	0.40
1:B:278:THR:C	1:B:280:ASN:N	2.75	0.40
1:B:261:PHE:HA	1:B:262:PRO:C	2.46	0.40
1:B:348:SER:HA	1:B:357:LYS:O	2.21	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	377/391 (96%)	361 (96%)	14 (4%)	2 (0%)	25	49
1	B	385/391 (98%)	360 (94%)	22 (6%)	3 (1%)	16	38
1	C	220/391 (56%)	200 (91%)	15 (7%)	5 (2%)	5	14
1	D	377/391 (96%)	356 (94%)	19 (5%)	2 (0%)	25	49
All	All	1359/1564 (87%)	1277 (94%)	70 (5%)	12 (1%)	14	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	PRO
1	B	93	ASN
1	B	279	GLY
1	C	118	PRO
1	C	172	ALA
1	D	118	PRO
1	A	46	ASP
1	D	172	ALA
1	C	352	ASP
1	B	46	ASP
1	C	340	PRO
1	C	88	ALA

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	308/319 (97%)	281 (91%)	27 (9%)	8	20
1	B	314/319 (98%)	288 (92%)	26 (8%)	9	22
1	C	175/319 (55%)	151 (86%)	24 (14%)	3	7
1	D	308/319 (97%)	280 (91%)	28 (9%)	7	19
All	All	1105/1276 (87%)	1000 (90%)	105 (10%)	7	17

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	31	GLN
1	A	47	VAL
1	A	48	ARG
1	A	70	THR
1	A	76	VAL
1	A	119	MET
1	A	127	THR
1	A	129	THR
1	A	133	LEU
1	A	158	THR
1	A	189	THR
1	A	208	VAL
1	A	220	THR
1	A	245	ILE
1	A	255	SER
1	A	281	THR
1	A	282	ILE
1	A	289	LEU
1	A	298	VAL
1	A	325	VAL
1	A	331	ASP
1	A	335	VAL
1	A	362	ARG
1	A	363	THR
1	A	365	ARG
1	A	372	VAL
1	B	5	MET
1	B	27	LEU
1	B	66	ILE
1	B	70	THR
1	B	76	VAL
1	B	86	THR

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Mol	Chain	Res	Type
1	B	119	MET
1	B	128	ASN
1	B	129	THR
1	B	136	GLU
1	B	145	LYS
1	B	158	THR
1	B	163	LEU
1	B	208	VAL
1	B	220	THR
1	B	222	ASP
1	B	235	GLU
1	B	250	THR
1	B	285	ASP
1	B	325	VAL
1	B	329	THR
1	B	335	VAL
1	B	344	ILE
1	B	363	THR
1	B	372	VAL
1	B	374	VAL
1	C	10	VAL
1	C	27	LEU
1	C	31	GLN
1	C	32	GLU
1	C	40	ARG
1	C	50	ILE
1	C	62	LYS
1	C	70	THR
1	C	114	LYS
1	C	127	THR
1	C	128	ASN
1	C	129	THR
1	C	145	LYS
1	C	158	THR
1	C	176	LYS
1	C	334	THR
1	C	335	VAL
1	C	343	VAL
1	C	348	SER
1	C	362	ARG
1	C	363	THR
1	C	372	VAL

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Mol	Chain	Res	Type
1	C	374	VAL
1	C	380	VAL
1	D	27	LEU
1	D	59	LEU
1	D	76	VAL
1	D	119	MET
1	D	127	THR
1	D	128	ASN
1	D	129	THR
1	D	174	THR
1	D	183	VAL
1	D	186	VAL
1	D	189	THR
1	D	208	VAL
1	D	220	THR
1	D	222	ASP
1	D	229	ASP
1	D	250	THR
1	D	268	THR
1	D	269	LYS
1	D	278	THR
1	D	289	LEU
1	D	298	VAL
1	D	325	VAL
1	D	335	VAL
1	D	344	ILE
1	D	357	LYS
1	D	360	LEU
1	D	363	THR
1	D	372	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	93	ASN
1	A	125	HIS
1	A	126	ASN
1	A	128	ASN
1	A	214	ASN
1	A	227	ASN
1	A	297	GLN

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Mol	Chain	Res	Type
1	A	324	GLN
1	B	125	HIS
1	B	126	ASN
1	B	128	ASN
1	C	31	GLN
1	C	71	HIS
1	C	125	HIS
1	C	126	ASN
1	C	128	ASN
1	D	71	HIS
1	D	95	ASN
1	D	125	HIS
1	D	126	ASN
1	D	128	ASN
1	D	227	ASN
1	D	280	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	379/391 (96%)	-0.36	1 (0%) 90 89	26, 43, 59, 68	0
1	B	387/391 (98%)	-0.14	4 (1%) 79 79	28, 48, 71, 84	0
1	C	224/391 (57%)	0.18	17 (7%) 21 19	32, 51, 100, 108	0
1	D	379/391 (96%)	-0.38	0 100 100	24, 39, 55, 61	0
All	All	1369/1564 (87%)	-0.21	22 (1%) 70 70	24, 44, 69, 108	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	ILE	5.9
1	C	350	VAL	5.7
1	C	337	ILE	5.4
1	C	343	VAL	4.7
1	C	352	ASP	4.6
1	C	335	VAL	4.3
1	C	340	PRO	3.8
1	C	346	VAL	3.8
1	C	341	ALA	3.6
1	C	334	THR	2.9
1	C	336	ARG	2.8
1	B	386	HIS	2.6
1	C	338	GLY	2.4
1	B	149	ASP	2.4
1	C	177	VAL	2.4
1	B	387	PRO	2.3
1	C	356	GLU	2.2
1	C	333	ASP	2.2
1	C	348	SER	2.2
1	B	119	MET	2.2
1	A	352	ASP	2.1
1	C	97	GLY	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.