



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DPZ
Title : STRUCTURE OF MODIFIED 3-ISOPROPYLMALATE DEHYDROGENASE
AT THE C-TERMINUS, HD711
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Deposited on : 1999-12-29
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

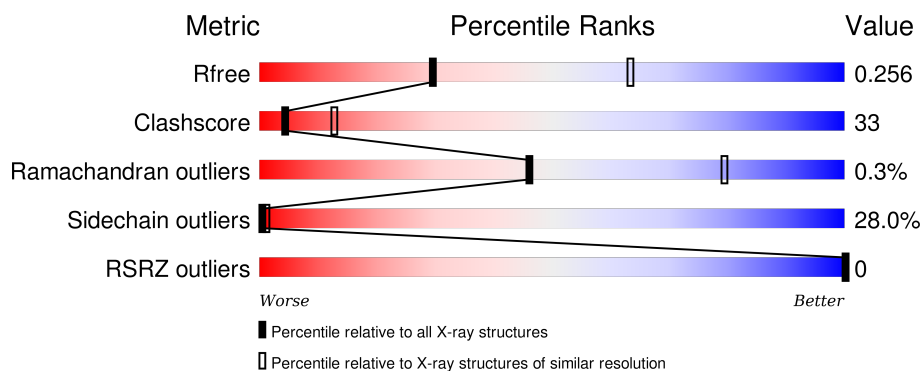
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	349	
1	B	349	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5248 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-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2592	1654	447	485	6			
1	B	344	Total	C	N	O	S	0	0	0
			2587	1651	446	484	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ARG	SER	SEE REMARK 999	UNP Q5SIY4
A	172	LEU	ALA	SEE REMARK 999	UNP Q5SIY4
A	341	GLU	LEU	SEE REMARK 999	UNP Q5SIY4
A	342	ALA	ARG	SEE REMARK 999	UNP Q5SIY4
A	343	PHE	HIS	SEE REMARK 999	UNP Q5SIY4
A	344	THR	LEU	SEE REMARK 999	UNP Q5SIY4
A	345	ALA	ALA	SEE REMARK 999	UNP Q5SIY4
A	346	THR	-	SEE REMARK 999	UNP Q5SIY4
A	347	VAL	-	SEE REMARK 999	UNP Q5SIY4
A	348	GLY	-	SEE REMARK 999	UNP Q5SIY4
A	349	ILE	-	SEE REMARK 999	UNP Q5SIY4
B	85	ARG	SER	SEE REMARK 999	UNP Q5SIY4
B	172	LEU	ALA	SEE REMARK 999	UNP Q5SIY4
B	341	GLU	LEU	SEE REMARK 999	UNP Q5SIY4
B	342	ALA	ARG	SEE REMARK 999	UNP Q5SIY4
B	343	PHE	HIS	SEE REMARK 999	UNP Q5SIY4
B	344	THR	LEU	SEE REMARK 999	UNP Q5SIY4
B	345	ALA	ALA	SEE REMARK 999	UNP Q5SIY4
B	346	THR	-	SEE REMARK 999	UNP Q5SIY4
B	347	VAL	-	SEE REMARK 999	UNP Q5SIY4
B	348	GLY	-	SEE REMARK 999	UNP Q5SIY4
B	349	ILE	-	SEE REMARK 999	UNP Q5SIY4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total 31	O 31	0	0
2	B	38	Total 38	O 38	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.43Å 87.57Å 70.89Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	6.80 – 2.80 36.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.6 (6.80-2.80) 57.6 (36.07-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.177 , 0.267 0.171 , 0.256	Depositor DCC
R_{free} test set	1332 reflections (10.04%)	DCC
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 19524 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5248	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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

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	0.40	0/2647	0.64	0/3594
1	B	0.39	0/2642	0.63	0/3587
All	All	0.40	0/5289	0.63	0/7181

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2592	0	2624	188	0
1	B	2587	0	2619	174	0
2	A	31	0	0	10	0
2	B	38	0	0	13	0
All	All	5248	0	5243	342	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 33.

All (342) 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:B:223:LEU:HB3	2:B:386:HOH:O	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG2	1:A:34:LEU:HA	1.48	0.96
1:A:164:ARG:HA	1:A:167:ARG:HD2	1.47	0.95
1:A:69:LEU:HB3	1:A:270:GLU:HB3	1.47	0.93
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.31	0.92
1:B:123:ALA:O	1:B:126:VAL:HG23	1.70	0.92
1:A:297:MET:SD	2:A:373:HOH:O	2.28	0.90
1:A:221:MET:HB2	1:B:249:VAL:HG11	1.52	0.89
1:A:297:MET:HB2	2:A:373:HOH:O	1.74	0.88
1:B:138:ILE:HB	1:B:155:GLU:HG2	1.55	0.88
1:A:248:SER:HB2	1:A:257:LEU:HD12	1.57	0.87
1:A:80:LEU:HD22	1:A:84:ILE:HD11	1.58	0.83
1:B:215:TYR:CD2	2:B:373:HOH:O	2.32	0.83
1:A:257:LEU:O	1:A:272:VAL:HG23	1.80	0.82
1:B:53:PHE:CE2	1:B:58:ARG:HG3	2.14	0.82
1:B:187:ASN:HB3	1:B:215:TYR:CZ	2.13	0.82
1:B:26:LEU:HD21	1:B:344:THR:OG1	1.80	0.81
1:A:143:PRO:O	1:A:154:THR:HG23	1.79	0.81
1:B:108:VAL:CG2	1:B:126:VAL:HB	2.12	0.80
1:B:143:PRO:O	1:B:154:THR:HG22	1.82	0.79
1:B:184:ASP:O	1:B:215:TYR:HA	1.83	0.77
1:B:215:TYR:HB2	2:B:373:HOH:O	1.82	0.77
1:B:215:TYR:HD2	2:B:373:HOH:O	1.63	0.77
1:B:22:VAL:O	1:B:26:LEU:HD23	1.85	0.76
1:A:245:ASP:OD2	1:B:217:ASP:HB2	1.85	0.75
1:A:309:ARG:NH1	1:A:309:ARG:HG2	1.96	0.73
1:A:80:LEU:HD23	1:A:81:PRO:HD2	1.70	0.73
1:B:108:VAL:HG23	1:B:126:VAL:HB	1.68	0.73
1:B:235:THR:HG21	2:B:384:HOH:O	1.87	0.73
1:A:187:ASN:HB3	1:A:215:TYR:CZ	2.23	0.72
1:B:298:LEU:HD22	1:B:304:LEU:HD12	1.70	0.71
1:A:290:ALA:CB	2:A:353:HOH:O	2.38	0.71
1:A:20:LEU:O	1:A:24:ARG:HG3	1.89	0.71
1:B:54:PRO:HB2	1:B:56:PRO:HD2	1.72	0.71
1:A:260:ALA:HB2	1:A:296:MET:HE3	1.73	0.71
1:B:26:LEU:HD12	1:B:307:LEU:HD21	1.71	0.71
1:B:118:LEU:HD13	1:B:122:ILE:HG22	1.73	0.71
1:B:193:GLU:O	1:B:197:LYS:HG2	1.91	0.70
1:A:297:MET:CB	2:A:373:HOH:O	2.33	0.70
1:A:248:SER:HB2	1:A:257:LEU:CD1	2.21	0.69
1:B:129:LEU:CD2	1:B:172:LEU:HD23	2.22	0.69
1:A:94:ARG:HA	1:A:99:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:MET:CG	2:A:373:HOH:O	2.38	0.69
1:B:99:LEU:HA	1:B:263:GLY:HA3	1.74	0.69
1:B:235:THR:CG2	2:B:384:HOH:O	2.40	0.68
1:A:85:ARG:O	1:A:88:THR:HG22	1.93	0.68
1:B:341:GLU:HA	1:B:344:THR:HG22	1.76	0.67
1:A:53:PHE:CZ	1:A:58:ARG:HA	2.30	0.67
1:A:282:LYS:HB3	1:A:284:ILE:HD13	1.77	0.67
1:A:194:PHE:CG	1:B:151:ALA:HB2	2.29	0.67
1:A:269:PHE:CE2	1:A:297:MET:HA	2.30	0.67
1:A:104:ARG:NH1	1:A:272:VAL:HG11	2.11	0.66
1:A:101:ALA:O	1:A:261:SER:HA	1.96	0.66
1:A:163:GLU:HB3	1:A:167:ARG:HE	1.61	0.66
1:B:159:LYS:O	1:B:163:GLU:HG2	1.94	0.66
1:A:164:ARG:CA	1:A:167:ARG:HD2	2.24	0.66
1:A:62:GLU:HG3	1:A:63:GLU:HG3	1.78	0.65
1:B:179:HIS:HE1	1:B:212:GLU:HG3	1.61	0.65
1:B:27:ASP:O	1:B:31:GLY:HA2	1.96	0.65
1:A:221:MET:HB2	1:B:249:VAL:CG1	2.26	0.65
1:B:115:LEU:HB3	1:B:252:GLY:HA3	1.76	0.65
1:B:138:ILE:HB	1:B:155:GLU:CG	2.27	0.65
1:B:97:GLN:HB3	1:B:99:LEU:HD21	1.79	0.65
1:A:156:ARG:HD3	1:B:150:GLU:OE1	1.96	0.65
1:B:286:ASN:HD22	1:B:287:PRO:HD2	1.62	0.65
1:A:223:LEU:O	1:A:227:PRO:HG3	1.98	0.64
1:A:5:VAL:C	1:A:6:LEU:HD12	2.17	0.64
1:B:286:ASN:ND2	1:B:288:THR:H	1.97	0.63
1:B:223:LEU:HD13	2:B:386:HOH:O	1.98	0.63
1:A:276:ALA:HB1	1:A:279:ILE:HD11	1.80	0.63
1:B:214:GLN:HE22	1:B:222:HIS:CD2	2.16	0.63
1:A:337:THR:HG22	1:A:341:GLU:OE1	1.98	0.63
1:B:235:THR:HG23	1:B:236:GLY:N	2.13	0.63
1:A:198:THR:O	1:A:202:VAL:HG23	1.99	0.63
1:B:211:LEU:HD23	1:B:212:GLU:H	1.65	0.62
1:B:260:ALA:HB2	1:B:296:MET:HE2	1.81	0.62
1:A:256:LEU:HG	1:A:288:THR:HG21	1.82	0.62
1:A:304:LEU:HB3	1:A:307:LEU:HB2	1.82	0.62
1:B:286:ASN:HD22	1:B:287:PRO:CD	2.12	0.62
1:A:256:LEU:C	1:A:257:LEU:HD23	2.21	0.60
1:A:256:LEU:HA	1:A:288:THR:HG22	1.83	0.60
1:A:99:LEU:HD22	1:A:261:SER:O	2.00	0.60
1:B:14:GLU:OE2	1:B:280:ALA:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:HG2	1:A:165:VAL:HG11	1.82	0.59
1:A:62:GLU:HG3	1:A:63:GLU:N	2.15	0.59
1:A:240:GLY:O	1:A:244:SER:OG	2.13	0.59
1:A:159:LYS:N	1:A:160:PRO:HD2	2.17	0.59
1:B:181:VAL:HG11	1:B:219:MET:CE	2.32	0.59
1:B:94:ARG:HD3	1:B:134:LEU:HD13	1.83	0.59
1:A:27:ASP:OD1	1:A:34:LEU:HB3	2.03	0.59
1:A:123:ALA:O	1:A:126:VAL:HG23	2.02	0.58
1:B:303:GLY:O	1:B:305:VAL:HG23	2.04	0.58
1:A:287:PRO:O	1:A:291:ILE:HG12	2.04	0.58
1:A:256:LEU:HA	1:A:288:THR:CG2	2.33	0.58
1:B:176:ARG:NH1	1:B:231:ASP:OD1	2.37	0.58
1:B:181:VAL:HG11	1:B:219:MET:HE1	1.86	0.58
1:A:276:ALA:N	1:A:277:PRO:HD3	2.19	0.57
1:A:184:ASP:OD1	1:A:196:ARG:NH1	2.38	0.57
1:B:158:SER:OG	1:B:160:PRO:HD2	2.05	0.57
1:A:191:VAL:HG23	1:B:153:ASN:OD1	2.05	0.57
1:A:309:ARG:CG	1:A:309:ARG:HH11	2.12	0.57
1:B:69:LEU:HB3	1:B:270:GLU:HB3	1.85	0.57
1:B:97:GLN:HG3	1:B:266:THR:N	2.20	0.57
1:A:26:LEU:HD22	1:A:307:LEU:HD13	1.86	0.56
1:B:129:LEU:HD21	1:B:172:LEU:HD23	1.85	0.56
1:A:196:ARG:NH2	1:A:213:HIS:HB3	2.20	0.56
1:A:158:SER:OG	1:A:161:GLU:HB2	2.05	0.56
1:A:102:ASN:HB2	1:A:134:LEU:HG	1.86	0.56
1:A:256:LEU:O	1:A:257:LEU:HD23	2.06	0.56
1:B:55:GLU:N	1:B:56:PRO:HD2	2.21	0.56
1:B:286:ASN:HD22	1:B:287:PRO:N	2.04	0.56
1:A:27:ASP:O	1:A:31:GLY:HA2	2.04	0.56
1:B:20:LEU:HD22	1:B:36:TYR:CE2	2.40	0.56
1:B:94:ARG:HD2	2:B:363:HOH:O	2.05	0.55
1:A:147:SER:OG	1:A:148:GLU:N	2.40	0.55
1:A:104:ARG:CZ	1:A:272:VAL:HG11	2.36	0.55
1:B:77:TRP:HA	1:B:80:LEU:HD13	1.88	0.55
1:A:221:MET:CE	1:B:249:VAL:HG12	2.37	0.55
1:B:26:LEU:HD12	1:B:307:LEU:CD2	2.37	0.55
1:A:191:VAL:CG2	1:B:153:ASN:HB2	2.35	0.55
1:A:187:ASN:OD1	1:A:188:VAL:HG22	2.06	0.55
1:A:142:GLU:OE2	1:A:143:PRO:HA	2.07	0.55
1:A:115:LEU:HD23	1:A:115:LEU:N	2.22	0.55
1:B:94:ARG:HD3	1:B:134:LEU:CD1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:O	1:A:167:ARG:HG3	2.07	0.54
1:A:196:ARG:HG3	1:A:213:HIS:ND1	2.22	0.54
1:B:250:LEU:HB2	1:B:251:PRO:HD3	1.89	0.54
1:B:116:SER:HB2	1:B:250:LEU:O	2.07	0.54
1:A:153:ASN:ND2	1:B:189:LEU:HB3	2.23	0.54
1:B:223:LEU:CB	2:B:386:HOH:O	2.34	0.54
1:B:235:THR:HG23	1:B:236:GLY:O	2.08	0.54
1:B:114:ARG:HG2	1:B:114:ARG:HH11	1.72	0.54
1:B:102:ASN:HB2	1:B:134:LEU:HG	1.90	0.54
1:A:221:MET:HE2	1:B:249:VAL:HG12	1.90	0.53
1:B:269:PHE:CD1	1:B:297:MET:HG3	2.43	0.53
1:A:102:ASN:HD22	1:A:132:ARG:NH1	2.07	0.53
1:A:92:SER:O	1:A:96:SER:HB3	2.09	0.53
1:A:269:PHE:CZ	1:A:297:MET:HA	2.43	0.53
1:B:272:VAL:CG1	1:B:272:VAL:O	2.57	0.53
1:A:206:TYR:N	1:A:207:PRO:HD3	2.24	0.53
1:B:190:GLU:N	1:B:190:GLU:OE1	2.42	0.53
1:A:103:LEU:HD21	1:A:172:LEU:HD21	1.90	0.52
1:A:279:ILE:HG22	1:A:284:ILE:HD11	1.91	0.52
1:A:194:PHE:CD1	1:B:151:ALA:HB2	2.44	0.52
1:A:55:GLU:N	1:A:56:PRO:HD2	2.24	0.52
1:B:159:LYS:N	1:B:160:PRO:HD2	2.24	0.52
1:B:5:VAL:HG21	1:B:20:LEU:HD21	1.91	0.52
1:B:255:GLY:O	1:B:289:ALA:HB2	2.10	0.52
1:A:98:ASP:OD2	1:A:264:ARG:HD2	2.09	0.52
1:B:200:GLU:HG3	1:B:213:HIS:NE2	2.25	0.52
1:B:27:ASP:HA	1:B:32:LEU:HD12	1.90	0.52
1:B:198:THR:O	1:B:202:VAL:HG13	2.10	0.52
1:A:325:PRO:HD3	1:A:331:ALA:O	2.10	0.52
1:A:143:PRO:HD2	1:A:154:THR:HG21	1.92	0.52
1:A:166:ALA:O	1:A:170:PHE:HD2	1.92	0.52
1:A:99:LEU:HA	1:A:263:GLY:HA3	1.92	0.51
1:A:282:LYS:O	1:A:284:ILE:HG23	2.10	0.51
1:B:6:LEU:CD1	1:B:39:PHE:HB2	2.41	0.51
1:A:260:ALA:HB2	1:A:296:MET:CE	2.38	0.51
1:A:174:ARG:HD2	1:A:206:TYR:HD2	1.74	0.51
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.76	0.51
1:A:165:VAL:HG23	1:A:166:ALA:N	2.26	0.51
1:A:187:ASN:HB3	1:A:215:TYR:OH	2.11	0.51
1:B:97:GLN:HB3	1:B:99:LEU:CD2	2.41	0.51
1:A:250:LEU:N	1:A:251:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:HE22	1:B:222:HIS:HD2	1.57	0.51
1:A:185:LYS:HG3	1:A:188:VAL:CG2	2.40	0.50
1:B:97:GLN:HG3	1:B:266:THR:H	1.75	0.50
1:A:307:LEU:O	1:A:310:LYS:HB3	2.11	0.50
1:A:32:LEU:HD22	1:A:32:LEU:H	1.75	0.50
1:A:290:ALA:HA	2:A:353:HOH:O	2.12	0.50
1:B:206:TYR:N	1:B:207:PRO:HD3	2.26	0.50
1:A:213:HIS:O	1:A:214:GLN:HG2	2.12	0.50
1:B:54:PRO:C	1:B:56:PRO:HD2	2.31	0.50
1:A:177:ARG:H	1:A:177:ARG:HD3	1.77	0.50
1:B:34:LEU:HD22	1:B:35:ALA:N	2.27	0.50
1:A:133:GLU:CG	1:A:165:VAL:HG11	2.41	0.49
1:B:114:ARG:CG	1:B:114:ARG:HH11	2.25	0.49
1:A:54:PRO:HB2	1:A:56:PRO:HD2	1.92	0.49
1:A:1:MET:HA	1:A:302:PHE:CE1	2.47	0.49
1:B:26:LEU:HD21	1:B:344:THR:CG2	2.43	0.49
1:B:90:LEU:HD22	1:B:94:ARG:NH2	2.26	0.49
1:B:248:SER:HB2	1:B:257:LEU:HD13	1.93	0.49
1:B:53:PHE:CZ	1:B:58:ARG:HA	2.48	0.49
1:A:177:ARG:NH2	1:A:230:PHE:O	2.44	0.49
1:B:187:ASN:OD1	1:B:188:VAL:HG23	2.13	0.49
1:A:343:PHE:N	1:A:343:PHE:CD1	2.79	0.49
1:A:186:ALA:HB3	1:A:196:ARG:NH1	2.28	0.49
1:A:82:ARG:HA	1:A:85:ARG:HD3	1.94	0.49
1:A:184:ASP:O	1:A:215:TYR:HA	2.12	0.49
1:B:59:LYS:HA	1:B:59:LYS:HD3	1.49	0.48
1:B:142:GLU:OE1	1:B:144:ARG:HG3	2.14	0.48
1:B:132:ARG:HB2	1:B:240:GLY:HA3	1.95	0.48
1:A:190:GLU:OE1	1:A:190:GLU:N	2.46	0.48
1:B:174:ARG:HD3	1:B:208:ASP:OD2	2.13	0.48
1:B:26:LEU:CD2	1:B:344:THR:OG1	2.59	0.48
1:B:115:LEU:HD21	1:B:327:LEU:HG	1.95	0.48
1:A:221:MET:HG3	1:A:225:ARG:HH21	1.79	0.48
1:A:191:VAL:HG21	1:B:153:ASN:HB2	1.96	0.48
1:A:290:ALA:HB1	2:A:353:HOH:O	2.08	0.47
1:B:6:LEU:HD11	1:B:39:PHE:HB2	1.95	0.47
1:B:155:GLU:OE2	1:B:191:VAL:HG11	2.14	0.47
1:B:26:LEU:CD2	1:B:26:LEU:N	2.77	0.47
1:A:226:SER:N	1:A:227:PRO:HD3	2.27	0.47
1:B:99:LEU:HD11	1:B:268:VAL:HG23	1.96	0.47
1:A:205:GLY:C	1:A:207:PRO:HD3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:CG	2:A:366:HOH:O	2.62	0.47
1:B:179:HIS:O	1:B:231:ASP:HB3	2.14	0.47
1:A:145:GLY:HA3	1:A:152:TRP:CZ2	2.50	0.47
1:A:164:ARG:CD	1:A:264:ARG:NH2	2.78	0.47
1:A:309:ARG:HD3	1:A:309:ARG:HA	1.52	0.47
1:A:248:SER:O	1:A:251:PRO:HD2	2.15	0.47
1:A:118:LEU:HD13	1:B:118:LEU:HD23	1.96	0.47
1:A:12:GLY:O	1:A:16:THR:HG23	2.15	0.47
1:A:302:PHE:HB3	1:A:304:LEU:HD23	1.97	0.47
1:B:238:ILE:CG2	1:B:239:PHE:N	2.78	0.47
1:B:275:SER:O	1:B:276:ALA:C	2.53	0.47
1:A:76:LYS:HG2	1:A:76:LYS:O	2.15	0.47
1:A:167:ARG:HG2	1:A:167:ARG:NH1	2.31	0.46
1:B:142:GLU:CG	1:B:143:PRO:HA	2.46	0.46
1:A:213:HIS:C	1:A:214:GLN:HG2	2.35	0.46
1:A:211:LEU:HD12	1:A:212:GLU:H	1.81	0.46
1:B:141:GLY:HA3	1:B:154:THR:O	2.15	0.46
1:A:276:ALA:N	1:A:277:PRO:CD	2.79	0.46
1:A:258:PRO:HG3	1:A:292:LEU:HB3	1.97	0.45
1:A:80:LEU:CD2	1:A:81:PRO:HD2	2.45	0.45
1:B:286:ASN:HD22	1:B:286:ASN:C	2.20	0.45
1:B:325:PRO:HA	1:B:329:GLY:O	2.15	0.45
1:B:26:LEU:HD11	1:B:344:THR:OG1	2.16	0.45
1:B:179:HIS:HB2	2:B:360:HOH:O	2.17	0.45
1:B:214:GLN:NE2	1:B:222:HIS:HD2	2.15	0.45
1:B:275:SER:HB2	1:B:277:PRO:HD3	1.97	0.45
1:B:103:LEU:N	1:B:103:LEU:HD12	2.31	0.45
1:A:153:ASN:HD22	1:B:189:LEU:HD22	1.81	0.45
1:B:138:ILE:CB	1:B:155:GLU:HG2	2.36	0.45
1:A:276:ALA:O	1:A:279:ILE:HG13	2.17	0.45
1:A:8:GLY:HA3	1:A:71:SER:O	2.17	0.45
1:A:27:ASP:HA	1:A:32:LEU:CD2	2.46	0.45
1:B:215:TYR:CB	2:B:373:HOH:O	2.53	0.45
1:B:298:LEU:CD2	1:B:304:LEU:HD12	2.44	0.45
1:B:216:VAL:HG13	1:B:217:ASP:N	2.32	0.45
1:B:199:VAL:HG12	1:B:211:LEU:HD11	1.98	0.44
1:A:40:PRO:CG	1:A:49:PHE:HE2	2.29	0.44
1:B:34:LEU:HD22	1:B:35:ALA:H	1.83	0.44
1:A:13:PRO:O	1:A:17:GLU:HB2	2.17	0.44
1:B:104:ARG:HB3	1:B:104:ARG:HE	1.71	0.44
1:A:6:LEU:O	1:A:69:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:PRO:N	1:B:154:THR:HG21	2.33	0.44
1:B:311:VAL:O	1:B:315:VAL:HG23	2.18	0.44
1:A:27:ASP:C	1:A:27:ASP:OD2	2.56	0.44
1:B:286:ASN:ND2	1:B:287:PRO:HD2	2.31	0.44
1:A:59:LYS:HA	1:A:62:GLU:HG2	1.99	0.44
1:A:195:TRP:O	1:A:199:VAL:HG23	2.18	0.44
1:A:189:LEU:CD2	1:B:138:ILE:HG12	2.47	0.44
1:B:304:LEU:HD12	1:B:307:LEU:HD12	2.00	0.44
1:B:159:LYS:H	1:B:160:PRO:HD2	1.82	0.44
1:A:185:LYS:HE2	1:A:187:ASN:OD1	2.18	0.43
1:B:112:LEU:HD12	1:B:114:ARG:CZ	2.48	0.43
1:A:276:ALA:CB	1:A:279:ILE:HD11	2.45	0.43
1:B:276:ALA:HB1	1:B:279:ILE:HG12	2.01	0.43
1:A:186:ALA:HB3	1:A:196:ARG:HH11	1.82	0.43
1:B:196:ARG:HE	1:B:196:ARG:HB2	1.50	0.43
1:B:143:PRO:CD	1:B:154:THR:HG21	2.48	0.43
1:B:240:GLY:HA2	2:B:384:HOH:O	2.19	0.43
1:B:55:GLU:N	1:B:56:PRO:CD	2.82	0.43
1:B:132:ARG:HH21	1:B:134:LEU:HD21	1.83	0.43
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.31	0.43
1:A:85:ARG:NH2	1:A:87:GLU:OE1	2.51	0.43
1:B:43:GLY:HA3	1:B:77:TRP:CZ2	2.54	0.43
1:B:247:ALA:HA	1:B:250:LEU:HD22	2.01	0.43
1:A:196:ARG:O	1:A:200:GLU:HB2	2.18	0.43
1:B:266:THR:HA	1:B:267:PRO:HD2	1.87	0.43
1:B:303:GLY:O	1:B:305:VAL:N	2.51	0.43
1:A:102:ASN:ND2	1:A:132:ARG:NH1	2.67	0.43
1:A:248:SER:HA	1:A:257:LEU:HD11	2.00	0.43
1:A:290:ALA:O	1:A:293:SER:HB2	2.19	0.43
1:A:297:MET:O	1:A:301:ALA:HB3	2.18	0.42
1:A:194:PHE:CB	1:B:151:ALA:HB2	2.48	0.42
1:A:112:LEU:HD22	1:A:115:LEU:HG	2.01	0.42
1:A:290:ALA:CA	2:A:353:HOH:O	2.65	0.42
1:B:259:SER:HB3	1:B:272:VAL:HG23	2.01	0.42
1:B:173:ALA:HB2	1:B:232:VAL:HG21	2.01	0.42
1:B:196:ARG:CZ	1:B:213:HIS:HB3	2.49	0.42
1:B:8:GLY:HA3	1:B:71:SER:O	2.19	0.42
1:A:164:ARG:HD2	1:A:264:ARG:NH2	2.35	0.42
1:A:11:ILE:HG12	1:A:276:ALA:HB3	2.00	0.42
1:B:158:SER:OG	1:B:160:PRO:HG2	2.19	0.42
1:B:43:GLY:O	1:B:46:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLY:O	1:B:144:ARG:HG2	2.20	0.42
1:A:113:GLU:H	1:A:113:GLU:CD	2.23	0.42
1:A:173:ALA:HB2	1:A:232:VAL:HG21	2.02	0.42
1:A:6:LEU:HD12	1:A:6:LEU:N	2.35	0.42
1:B:272:VAL:HG12	1:B:272:VAL:O	2.18	0.42
1:A:174:ARG:HD2	1:A:206:TYR:CD2	2.53	0.42
1:B:82:ARG:O	1:B:82:ARG:HG2	2.15	0.42
1:B:158:SER:OG	1:B:160:PRO:CD	2.67	0.42
1:A:310:LYS:CD	2:A:366:HOH:O	2.68	0.42
1:A:69:LEU:HD12	1:A:70:GLY:H	1.85	0.42
1:B:211:LEU:HD23	1:B:212:GLU:N	2.31	0.42
1:A:238:ILE:HG23	1:A:239:PHE:N	2.34	0.42
1:A:335:ALA:O	1:A:338:ALA:HB3	2.20	0.42
1:B:304:LEU:N	1:B:304:LEU:HD23	2.35	0.41
1:B:243:LEU:HD12	2:B:384:HOH:O	2.20	0.41
1:A:159:LYS:N	1:A:160:PRO:CD	2.82	0.41
1:B:142:GLU:HG3	1:B:143:PRO:HA	2.02	0.41
1:A:287:PRO:O	1:A:290:ALA:HB3	2.19	0.41
1:A:2:LYS:H	1:A:65:GLU:HG3	1.84	0.41
1:A:163:GLU:OE2	1:A:167:ARG:NH2	2.51	0.41
1:B:112:LEU:HA	1:B:112:LEU:HD12	1.79	0.41
1:A:118:LEU:CD1	1:B:118:LEU:HD23	2.50	0.41
1:B:103:LEU:CD1	1:B:103:LEU:N	2.84	0.41
1:A:49:PHE:CD2	1:A:54:PRO:HG3	2.56	0.41
1:A:5:VAL:O	1:A:6:LEU:HD12	2.21	0.41
1:B:307:LEU:O	1:B:310:LYS:HB3	2.21	0.41
1:A:27:ASP:HA	1:A:32:LEU:HD22	2.03	0.41
1:A:163:GLU:HB3	1:A:167:ARG:NE	2.34	0.41
1:A:189:LEU:HD22	1:B:138:ILE:HG12	2.02	0.41
1:B:213:HIS:O	1:B:214:GLN:HG2	2.21	0.41
1:A:174:ARG:O	1:A:178:LYS:HE3	2.21	0.41
1:A:27:ASP:O	1:A:31:GLY:N	2.53	0.41
1:A:164:ARG:HD3	1:A:264:ARG:NH2	2.36	0.41
1:A:249:VAL:C	1:A:251:PRO:HD2	2.40	0.41
1:A:171:GLU:OE1	1:A:206:TYR:HE2	2.04	0.41
1:B:238:ILE:HD13	1:B:238:ILE:O	2.20	0.41
1:A:212:GLU:CD	1:A:229:ARG:HH22	2.24	0.41
1:B:121:GLU:CD	1:B:121:GLU:H	2.24	0.41
1:B:142:GLU:CD	1:B:143:PRO:HA	2.41	0.41
1:A:154:THR:HA	1:B:154:THR:HA	2.03	0.41
1:A:303:GLY:O	1:A:305:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:PHE:CD1	1:A:269:PHE:N	2.89	0.40
1:A:286:ASN:HD22	1:A:287:PRO:HD2	1.86	0.40
1:A:211:LEU:HD12	1:A:212:GLU:N	2.36	0.40
1:B:186:ALA:HB2	1:B:192:GLY:O	2.21	0.40
1:A:218:ALA:O	1:A:221:MET:HG2	2.21	0.40
1:A:112:LEU:HD22	1:A:115:LEU:CG	2.51	0.40
1:A:119:LYS:HB2	1:A:122:ILE:HG13	2.04	0.40
1:B:143:PRO:HD2	1:B:154:THR:HG21	2.03	0.40
1:B:296:MET:HB3	1:B:296:MET:HE2	1.97	0.40
1:A:69:LEU:HB3	1:A:270:GLU:CB	2.35	0.40
1:B:143:PRO:O	1:B:154:THR:CG2	2.61	0.40
1:B:187:ASN:HB3	1:B:215:TYR:CE2	2.55	0.40
1:A:155:GLU:N	1:B:153:ASN:O	2.48	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	343/349 (98%)	316 (92%)	27 (8%)	0	100	100
1	B	342/349 (98%)	314 (92%)	26 (8%)	2 (1%)	30	65
All	All	685/698 (98%)	630 (92%)	53 (8%)	2 (0%)	46	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	GLY
1	B	321	GLU

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	266 / 269 (99%)	192 (72%)	74 (28%)	0	1
1	B	266 / 269 (99%)	191 (72%)	75 (28%)	0	1
All	All	532 / 538 (99%)	383 (72%)	149 (28%)	0	1

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	9	ASP
1	A	11	ILE
1	A	14	GLU
1	A	23	LEU
1	A	32	LEU
1	A	38	VAL
1	A	51	GLU
1	A	58	ARG
1	A	59	LYS
1	A	61	VAL
1	A	62	GLU
1	A	65	GLU
1	A	68	LEU
1	A	72	VAL
1	A	82	ARG
1	A	85	ARG
1	A	87	GLU
1	A	90	LEU
1	A	91	LEU
1	A	94	ARG
1	A	96	SER
1	A	112	LEU
1	A	114	ARG
1	A	115	LEU
1	A	118	LEU
1	A	120	GLU

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Mol	Chain	Res	Type
1	A	121	GLU
1	A	128	VAL
1	A	150	GLU
1	A	154	THR
1	A	155	GLU
1	A	159	LYS
1	A	164	ARG
1	A	167	ARG
1	A	171	GLU
1	A	172	LEU
1	A	175	LYS
1	A	185	LYS
1	A	188	VAL
1	A	191	VAL
1	A	196	ARG
1	A	197	LYS
1	A	223	LEU
1	A	225	ARG
1	A	226	SER
1	A	229	ARG
1	A	238	ILE
1	A	241	ASP
1	A	248	SER
1	A	249	VAL
1	A	250	LEU
1	A	253	SER
1	A	254	LEU
1	A	256	LEU
1	A	262	LEU
1	A	264	ARG
1	A	266	THR
1	A	275	SER
1	A	279	ILE
1	A	282	LYS
1	A	284	ILE
1	A	288	THR
1	A	297	MET
1	A	299	GLU
1	A	307	LEU
1	A	309	ARG
1	A	310	LYS
1	A	320	LEU

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Mol	Chain	Res	Type
1	A	321	GLU
1	A	327	LEU
1	A	334	GLU
1	A	341	GLU
1	A	343	PHE
1	B	6	LEU
1	B	21	LYS
1	B	23	LEU
1	B	26	LEU
1	B	30	GLU
1	B	32	LEU
1	B	34	LEU
1	B	51	GLU
1	B	55	GLU
1	B	58	ARG
1	B	59	LYS
1	B	62	GLU
1	B	68	LEU
1	B	69	LEU
1	B	72	VAL
1	B	82	ARG
1	B	85	ARG
1	B	91	LEU
1	B	92	SER
1	B	93	LEU
1	B	97	GLN
1	B	107	LYS
1	B	108	VAL
1	B	112	LEU
1	B	114	ARG
1	B	116	SER
1	B	120	GLU
1	B	132	ARG
1	B	144	ARG
1	B	147	SER
1	B	148	GLU
1	B	150	GLU
1	B	154	THR
1	B	155	GLU
1	B	156	ARG
1	B	157	TYR
1	B	158	SER

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Mol	Chain	Res	Type
1	B	159	LYS
1	B	163	GLU
1	B	164	ARG
1	B	174	ARG
1	B	175	LYS
1	B	178	LYS
1	B	193	GLU
1	B	196	ARG
1	B	197	LYS
1	B	201	GLU
1	B	202	VAL
1	B	211	LEU
1	B	221	MET
1	B	226	SER
1	B	229	ARG
1	B	235	THR
1	B	238	ILE
1	B	241	ASP
1	B	245	ASP
1	B	249	VAL
1	B	250	LEU
1	B	253	SER
1	B	254	LEU
1	B	262	LEU
1	B	264	ARG
1	B	275	SER
1	B	282	LYS
1	B	286	ASN
1	B	297	MET
1	B	304	LEU
1	B	307	LEU
1	B	309	ARG
1	B	313	ASP
1	B	321	GLU
1	B	322	THR
1	B	327	LEU
1	B	330	SER
1	B	337	THR

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	102	ASN
1	A	153	ASN
1	A	286	ASN
1	B	222	HIS
1	B	286	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	345/349 (98%)	-0.76	0 100 100	11, 39, 59, 83	0
1	B	344/349 (98%)	-0.81	0 100 100	11, 39, 54, 64	0
All	All	689/698 (98%)	-0.78	0 100 100	11, 39, 57, 83	0

There are no RSRZ outliers to report.

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.