Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 06:04 PM EST

PDB ID	:	2GF2
Title	:	Crystal structure of human hydroxyisobutyrate dehydrogenase
Authors	:	Papagrigoriou, E.; Salah, E.; Turnbull, A.P.; Smee, C.; Burgess, N.; Gileadi, O.; von Delft, F.; Gorrec, F.; Arrowsmith, C.H.; Weigelt, J.; Sundstrom, M.; Edwards, A.M.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-03-21
Resolution	:	2.38 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:

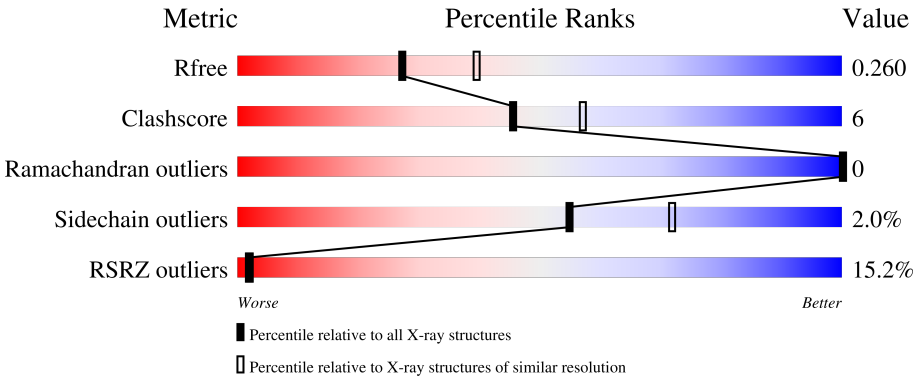
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.38 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	296	86% 13%
1	B	296	2% 85% 13%
1	C	296	30% 86% 12%
1	D	296	28% 86% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8774 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-hydroxyisobutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2152	1353	359	418	22			
1	B	293	Total	C	N	O	S	0	0	0
			2116	1339	351	404	22			
1	C	291	Total	C	N	O	S	0	0	0
			2093	1325	349	397	22			
1	D	294	Total	C	N	O	S	0	1	0
			2130	1347	354	406	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	initiating methionine	UNP P31937
B	40	MET	-	initiating methionine	UNP P31937
C	40	MET	-	initiating methionine	UNP P31937
D	40	MET	-	initiating methionine	UNP P31937

- Molecule 2 is water.

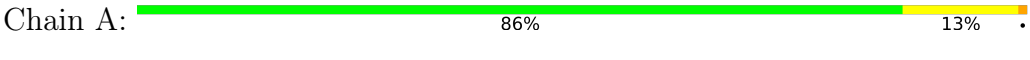
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	77	Total	O	0	1
			78	78		
2	B	73	Total	O	0	5
			79	79		
2	C	62	Total	O	0	2
			64	64		
2	D	61	Total	O	0	1
			62	62		

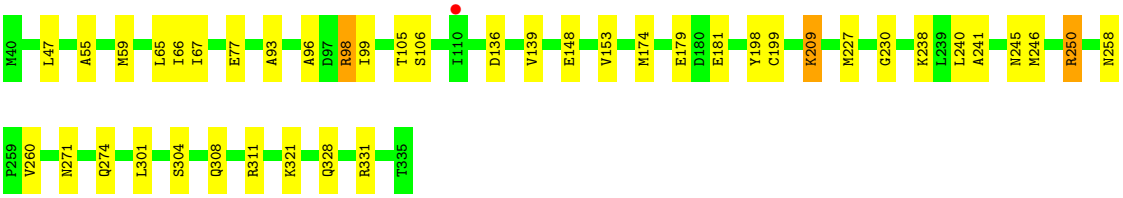
3 Residue-property plots (i)

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-hydroxyisobutyrate dehydrogenase

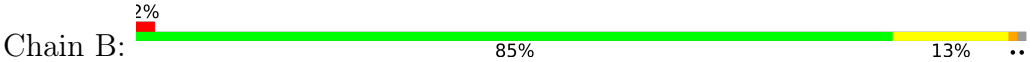
Chain A:

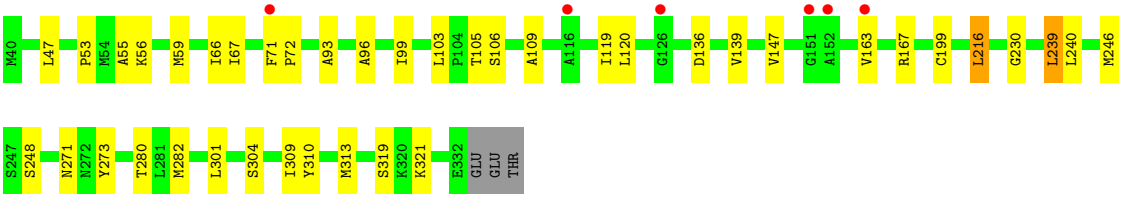




• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

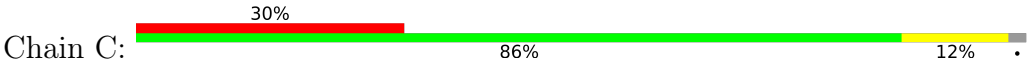
Chain B:

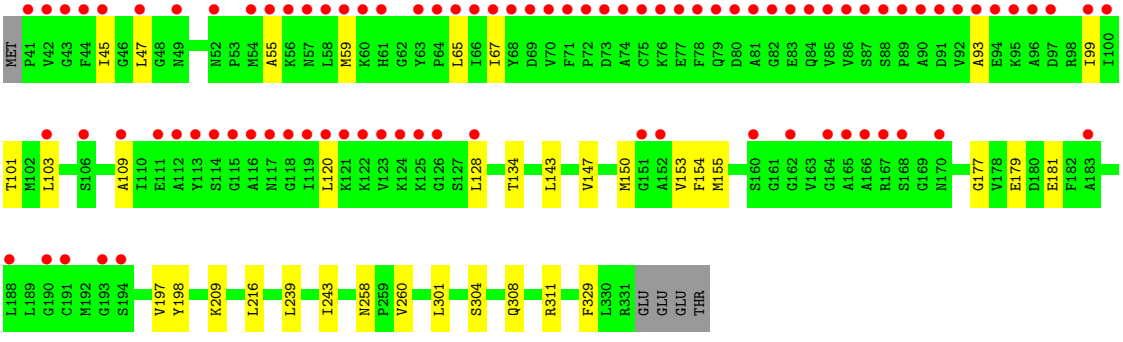




• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

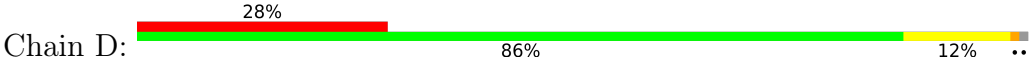
Chain C:

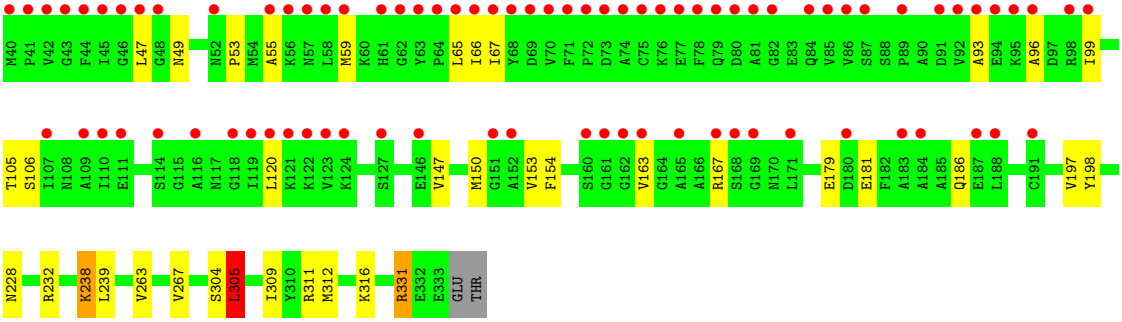




• Molecule 1: 3-hydroxyisobutyrate dehydrogenase

Chain D:




M40 P41 V42 G43 F44 I45 G46 L47 G48 N49 N52 P53 M54 A55 K56 N57 L58 M59 K60 H61 G62 Y63 P64 L65 I66 I67 Y68 D69 V70 F71 P72 D73 A74 C75 K76 E77 F78 Q79 D80 A81 G82 E83 Q84 V85 V86 S87 S88 P89 A90 D91 V92 A93 E94 K95 A96 D97 R98 I99
T105 S106 I107 N108 A109 I110 E111 S114 G115 A116 N117 G118 I119 L120 K121 K122 V123 K124 S127 E146 V147 M150 G151 A152 V153 F154 S160 G161 G162 V163 G164 A165 A166 R167 S168 G169 N170 L171 E179 D180 E181 F182 A183 A184 A185 Q186 E187 L188 C191 V197 Y198
N228 R232 K238 L239 V263 V267 S304 L305 I309 Y310 R311 M312 K316 R331 E332 E333 GLU THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.05Å 122.75Å 200.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.38 48.56 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.56-2.38) 99.4 (48.56-2.38)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.247 0.229 , 0.260	Depositor DCC
R_{free} test set	2625 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8774	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

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	0.48	0/2187	0.60	0/2954
1	B	0.46	1/2150 (0.0%)	0.58	0/2904
1	C	0.41	0/2127	0.56	0/2871
1	D	0.45	1/2167 (0.0%)	0.57	1/2926 (0.0%)
All	All	0.45	2/8631 (0.0%)	0.58	1/11655 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	ILE	C-N	-5.17	1.22	1.34
1	D	267	VAL	C-N	-5.10	1.24	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	305	LEU	CA-CB-CG	5.19	127.24	115.30

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	2152	0	2135	36	0
1	B	2116	0	2116	33	0
1	C	2093	0	2097	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2130	0	2135	29	0
2	A	78	0	0	4	0
2	B	79	0	0	1	0
2	C	64	0	0	1	0
2	D	62	0	0	1	0
All	All	8774	0	8483	109	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 6.

All (109) 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:174:MET:HE2	2:A:382:HOH:O	1.58	0.99
1:D:331:ARG:HH21	1:D:331:ARG:HG3	1.37	0.89
1:B:309:ILE:HG22	1:B:313:MET:HE2	1.58	0.84
1:C:153:VAL:HG21	1:C:181:GLU:HG3	1.60	0.82
1:A:174:MET:HE3	1:A:209:LYS:HB2	1.67	0.77
1:D:147:VAL:HG21	1:D:154:PHE:HB2	1.64	0.77
1:B:246:MET:CE	1:C:197:VAL:HG21	2.16	0.76
1:D:331:ARG:HH21	1:D:331:ARG:CG	1.99	0.75
1:B:309:ILE:HG22	1:B:313:MET:CE	2.19	0.72
1:A:174:MET:CE	1:A:209:LYS:HB2	2.20	0.72
1:B:216:LEU:HD13	1:B:282:MET:HE1	1.76	0.67
1:A:301:LEU:HD23	1:C:308:GLN:HB3	1.75	0.67
1:B:163:VAL:O	1:B:167:ARG:HG3	1.94	0.67
1:B:246:MET:HE1	1:C:197:VAL:HG21	1.77	0.66
1:B:309:ILE:CG2	1:B:313:MET:HE2	2.27	0.65
1:A:98:ARG:HH21	1:A:98:ARG:HG2	1.62	0.65
1:A:179:GLU:HB3	1:A:198:TYR:CZ	2.35	0.62
1:D:47:LEU:HD11	1:D:67:ILE:CG2	2.29	0.62
1:A:47:LEU:HD11	1:A:67:ILE:CG2	2.31	0.60
1:B:246:MET:HE3	1:C:197:VAL:HG21	1.82	0.60
1:B:47:LEU:HD11	1:B:67:ILE:CG2	2.32	0.60
1:D:312:MET:O	1:D:316:LYS:HG2	2.01	0.60
1:B:136:ASP:HB3	1:B:139:VAL:HG23	1.83	0.59
1:C:47:LEU:HD11	1:C:67:ILE:CG2	2.31	0.59
1:C:147:VAL:HG21	1:C:154:PHE:HB2	1.85	0.58
1:A:174:MET:CE	2:A:382:HOH:O	2.33	0.58
1:B:310:TYR:HA	1:B:313:MET:HE3	1.87	0.57
1:A:136:ASP:HB3	1:A:139:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG11	1:A:181:GLU:HG3	1.86	0.56
1:B:105:THR:HG22	1:B:106:SER:N	2.20	0.56
1:A:301:LEU:HD23	1:C:308:GLN:CB	2.35	0.55
1:B:199:CYS:HA	1:C:239:LEU:CD2	2.36	0.55
1:A:199:CYS:HA	1:D:239:LEU:HD21	1.88	0.55
1:D:47:LEU:HD11	1:D:67:ILE:HG23	1.89	0.54
1:A:98:ARG:HH21	1:A:98:ARG:CG	2.19	0.54
1:B:199:CYS:HA	1:C:239:LEU:HD21	1.89	0.54
1:D:311:ARG:HD2	2:D:340:HOH:O	2.07	0.54
1:B:47:LEU:HD11	1:B:67:ILE:HG23	1.90	0.54
1:A:47:LEU:HD11	1:A:67:ILE:HG23	1.90	0.53
1:C:134:THR:OG1	1:C:209:LYS:NZ	2.40	0.53
1:C:329:PHE:O	1:D:316:LYS:NZ	2.39	0.53
1:A:77:GLU:HB2	2:A:353:HOH:O	2.08	0.53
1:C:47:LEU:HD11	1:C:67:ILE:HG23	1.91	0.52
1:A:246:MET:CE	1:D:197:VAL:HG21	2.39	0.52
1:C:179:GLU:HB3	1:C:198:TYR:CZ	2.44	0.52
1:D:120:LEU:HD11	1:D:147:VAL:HG12	1.93	0.51
1:A:301:LEU:HD12	1:D:309:ILE:HD11	1.93	0.51
1:A:245:ASN:HB3	1:A:250[A]:ARG:HH11	1.76	0.51
1:D:153:VAL:HG21	1:D:181:GLU:HG3	1.93	0.50
1:D:93:ALA:HA	1:D:99:ILE:HD11	1.92	0.50
1:D:331:ARG:CG	1:D:331:ARG:NH2	2.65	0.50
1:B:199:CYS:SG	1:C:243:ILE:HD11	2.52	0.49
1:A:105:THR:HG22	1:A:106:SER:N	2.28	0.49
1:B:273:TYR:HB2	1:B:321:LYS:HE3	1.94	0.49
1:D:147:VAL:CG2	1:D:154:PHE:HB2	2.41	0.49
1:C:93:ALA:HA	1:C:99:ILE:HD11	1.94	0.49
1:A:93:ALA:HA	1:A:99:ILE:HD11	1.94	0.49
1:B:248:SER:OG	1:C:216:LEU:HD22	2.12	0.49
1:A:258:ASN:HD22	1:A:260:VAL:H	1.60	0.48
1:D:163:VAL:HG12	1:D:167:ARG:HH11	1.79	0.48
1:A:55:ALA:O	1:A:59:MET:HG3	2.14	0.48
1:D:238:LYS:HE2	1:D:263:VAL:O	2.13	0.47
1:A:301:LEU:CD2	1:C:308:GLN:CB	2.92	0.47
1:B:93:ALA:HA	1:B:99:ILE:HD11	1.95	0.47
1:A:230:GLY:HA3	1:A:240:LEU:HD22	1.95	0.47
1:C:258:ASN:HD22	1:C:260:VAL:H	1.61	0.47
1:D:53:PRO:HB3	1:D:167:ARG:HG3	1.97	0.47
1:B:120:LEU:HD21	1:B:147:VAL:HG22	1.97	0.47
1:B:321:LYS:HE2	2:B:366:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD23	1:A:67:ILE:HD11	1.97	0.46
1:C:311:ARG:HD2	2:C:345:HOH:O	2.16	0.46
1:A:246:MET:HE1	1:D:197:VAL:HG21	1.98	0.46
1:B:53:PRO:HB3	1:B:167:ARG:HG2	1.97	0.46
1:A:311:ARG:HD2	2:A:405:HOH:O	2.16	0.45
1:C:103:LEU:HD13	1:C:109:ALA:HA	1.98	0.45
1:A:98:ARG:CG	1:A:98:ARG:NH2	2.78	0.45
1:B:103:LEU:HD13	1:B:109:ALA:HA	1.99	0.45
1:B:280:THR:OG1	1:B:319:SER:HB2	2.16	0.45
1:B:66:ILE:HD12	1:B:96:ALA:HB2	1.99	0.45
1:C:155:MET:HE2	1:C:177:GLY:HA3	1.99	0.45
1:A:271:ASN:O	1:A:274:GLN:HG2	2.17	0.44
1:B:304:SER:HB3	1:D:304:SER:HB3	1.99	0.44
1:D:55:ALA:O	1:D:59:MET:HG3	2.18	0.44
1:B:239:LEU:O	1:B:239:LEU:HG	2.09	0.44
1:C:65:LEU:HD23	1:C:67:ILE:HD11	2.00	0.44
1:C:304:SER:O	1:C:308:GLN:HG2	2.16	0.44
1:D:228:ASN:O	1:D:232:ARG:HG3	2.17	0.44
1:A:227:MET:HE1	1:A:241:ALA:HA	2.00	0.44
1:A:304:SER:HB3	1:C:304:SER:HB3	1.99	0.44
1:C:55:ALA:O	1:C:59:MET:HG3	2.18	0.44
1:C:155:MET:CE	1:C:177:GLY:HA3	2.48	0.44
1:D:238:LYS:CE	1:D:263:VAL:O	2.66	0.44
1:D:105:THR:HG22	1:D:106:SER:N	2.33	0.43
1:A:301:LEU:CD2	1:C:308:GLN:HB2	2.48	0.43
1:D:65:LEU:HD23	1:D:67:ILE:HD11	1.99	0.43
1:A:301:LEU:CD2	1:C:308:GLN:HB3	2.45	0.43
1:B:55:ALA:O	1:B:59:MET:HG3	2.19	0.43
1:B:301:LEU:HD22	1:D:305:LEU:CD1	2.49	0.42
1:D:179:GLU:HB3	1:D:198:TYR:CZ	2.55	0.42
1:D:66:ILE:HD12	1:D:96:ALA:HB2	2.01	0.42
1:A:66:ILE:HD12	1:A:96:ALA:HB2	2.02	0.41
1:B:105:THR:CG2	1:B:106:SER:N	2.83	0.41
1:B:230:GLY:HA3	1:B:240:LEU:HD22	2.03	0.41
1:A:308:GLN:HB2	1:C:301:LEU:HD23	2.02	0.41
1:B:56:LYS:HA	1:B:59:MET:HE2	2.03	0.41
1:C:143:LEU:O	1:C:147:VAL:HG13	2.20	0.41
1:C:45:ILE:HB	1:C:101:THR:HG22	2.03	0.40
1:A:321:LYS:HE2	1:A:328:GLN:OE1	2.20	0.40
1:B:71:PHE:HA	1:B:72:PRO:HD2	1.99	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	295/296 (100%)	288 (98%)	7 (2%)	0	100	100
1	B	291/296 (98%)	284 (98%)	7 (2%)	0	100	100
1	C	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
1	D	293/296 (99%)	288 (98%)	5 (2%)	0	100	100
All	All	1168/1184 (99%)	1143 (98%)	25 (2%)	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	225/232 (97%)	218 (97%)	7 (3%)	40	57
1	B	219/232 (94%)	216 (99%)	3 (1%)	67	81
1	C	216/232 (93%)	213 (99%)	3 (1%)	67	81
1	D	222/232 (96%)	216 (97%)	6 (3%)	44	62
All	All	882/928 (95%)	863 (98%)	19 (2%)	55	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ARG
1	A	148	GLU

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Mol	Chain	Res	Type
1	A	209	LYS
1	A	238	LYS
1	A	250[A]	ARG
1	A	250[B]	ARG
1	A	331	ARG
1	B	216	LEU
1	B	239	LEU
1	B	271	ASN
1	C	120	LEU
1	C	128	LEU
1	C	150	MET
1	D	49	ASN
1	D	150	MET
1	D	186	GLN
1	D	238	LYS
1	D	305	LEU
1	D	331	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	296/296 (100%)	0.26	1 (0%) 94 94	20, 33, 49, 56	0
1	B	293/296 (98%)	0.24	6 (2%) 65 66	21, 33, 50, 57	0
1	C	291/296 (98%)	1.40	89 (30%) 0 0	21, 38, 54, 56	0
1	D	294/296 (99%)	1.30	82 (27%) 0 0	21, 38, 55, 57	0
All	All	1174/1184 (99%)	0.80	178 (15%) 2 2	20, 34, 54, 57	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	78	PHE	10.3
1	D	75	CYS	9.1
1	C	75	CYS	8.9
1	D	71	PHE	8.1
1	D	40	MET	7.9
1	C	44	PHE	7.5
1	C	74	ALA	7.4
1	D	70	VAL	7.2
1	D	78	PHE	7.2
1	D	120	LEU	6.6
1	D	66	ILE	6.6
1	D	82	GLY	6.5
1	D	81	ALA	6.2
1	D	62	GLY	6.0
1	D	65	LEU	6.0
1	C	69	ASP	5.9
1	C	58	LEU	5.8
1	D	72	PRO	5.6
1	C	86	VAL	5.6
1	D	84	GLN	5.6
1	C	88	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	79	GLN	5.6
1	D	188	LEU	5.5
1	C	68	TYR	5.5
1	D	121	LYS	5.4
1	C	92	VAL	5.4
1	D	59	MET	5.4
1	C	65	LEU	5.3
1	D	124	LYS	5.3
1	C	82	GLY	5.3
1	D	41	PRO	5.3
1	C	66	ILE	5.3
1	C	123	VAL	5.2
1	C	41	PRO	5.2
1	C	116	ALA	5.1
1	D	73	ASP	5.1
1	D	63	TYR	5.1
1	D	67	ILE	5.0
1	D	86	VAL	4.9
1	D	47	LEU	4.9
1	D	95	LYS	4.9
1	D	74	ALA	4.8
1	C	166	ALA	4.7
1	C	47	LEU	4.7
1	C	95	LYS	4.6
1	C	118	GLY	4.6
1	C	56	LYS	4.5
1	D	55	ALA	4.5
1	D	92	VAL	4.4
1	D	68	TYR	4.4
1	C	84	GLN	4.3
1	C	122	LYS	4.3
1	C	85	VAL	4.3
1	D	123	VAL	4.3
1	C	71	PHE	4.3
1	C	80	ASP	4.2
1	C	165	ALA	4.2
1	D	107	ILE	4.2
1	C	90	ALA	4.2
1	C	124	LYS	4.2
1	C	87	SER	4.1
1	C	117	ASN	4.0
1	D	94	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	64	PRO	4.0
1	D	96	ALA	3.9
1	C	162	GLY	3.9
1	C	120	LEU	3.9
1	D	87	SER	3.9
1	D	118	GLY	3.9
1	B	116	ALA	3.9
1	C	67	ILE	3.9
1	D	168	SER	3.9
1	D	99	ILE	3.8
1	C	121	LYS	3.8
1	D	85	VAL	3.8
1	C	45	ILE	3.8
1	C	54	MET	3.8
1	C	60	LYS	3.7
1	D	122	LYS	3.7
1	D	80	ASP	3.7
1	C	152	ALA	3.7
1	C	89	PRO	3.7
1	C	73	ASP	3.6
1	C	70	VAL	3.5
1	C	115	GLY	3.5
1	C	188	LEU	3.5
1	C	94	GLU	3.5
1	C	96	ALA	3.5
1	D	89	PRO	3.5
1	C	57	ASN	3.5
1	C	194	SER	3.5
1	C	119	ILE	3.5
1	C	64	PRO	3.5
1	C	72	PRO	3.4
1	D	42	VAL	3.4
1	D	184	ALA	3.4
1	D	187	GLU	3.4
1	D	163	VAL	3.3
1	C	79	GLN	3.3
1	D	160	SER	3.3
1	C	113	TYR	3.2
1	C	97	ASP	3.2
1	D	58	LEU	3.2
1	D	61	HIS	3.2
1	C	183	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	77	GLU	3.2
1	C	93	ALA	3.1
1	C	125	LYS	3.1
1	B	71	PHE	3.1
1	C	61	HIS	3.1
1	C	167	ARG	3.0
1	D	44	PHE	3.0
1	D	110	ILE	3.0
1	D	91	ASP	3.0
1	C	170	ASN	3.0
1	C	43	GLY	2.9
1	C	99	ILE	2.9
1	C	111	GLU	2.9
1	C	81	ALA	2.9
1	D	152	ALA	2.9
1	C	191	CYS	2.9
1	D	69	ASP	2.8
1	D	167	ARG	2.8
1	D	57	ASN	2.8
1	C	91	ASP	2.8
1	D	111	GLU	2.8
1	D	52	ASN	2.8
1	C	126	GLY	2.8
1	D	116	ALA	2.7
1	C	190	GLY	2.7
1	C	52	ASN	2.7
1	D	43	GLY	2.7
1	B	163	VAL	2.6
1	C	160	SER	2.6
1	D	171	LEU	2.6
1	C	42	VAL	2.6
1	B	151	GLY	2.6
1	C	100	ILE	2.6
1	D	127	SER	2.5
1	C	55	ALA	2.5
1	D	56	LYS	2.5
1	B	152	ALA	2.5
1	C	76	LYS	2.5
1	C	109	ALA	2.5
1	C	63	TYR	2.5
1	D	76	LYS	2.5
1	B	126	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	164	GLY	2.5
1	D	93	ALA	2.4
1	D	45	ILE	2.4
1	D	191	CYS	2.4
1	C	168	SER	2.4
1	D	46	GLY	2.4
1	D	162	GLY	2.4
1	A	110	ILE	2.3
1	D	151	GLY	2.3
1	C	59	MET	2.3
1	D	119	ILE	2.3
1	D	165	ALA	2.3
1	C	103	LEU	2.2
1	C	151	GLY	2.2
1	D	109	ALA	2.2
1	D	146	GLU	2.2
1	C	114	SER	2.2
1	D	114	SER	2.2
1	C	49	ASN	2.1
1	C	106	SER	2.1
1	D	180	ASP	2.1
1	D	161	GLY	2.1
1	D	169	GLY	2.1
1	C	193	GLY	2.1
1	C	112	ALA	2.1
1	C	83	GLU	2.1
1	C	128	LEU	2.1
1	D	77	GLU	2.1
1	D	48	GLY	2.1
1	D	98	ARG	2.1
1	D	183	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.