Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:41 pm BST

PDB ID	:	1U2E
Title	:	Crystal Structure of the C-C bond hydrolase MhpC
Authors	:	Montgomery, M.G.; Dunn, G.; Mohammed, F.; Robertson, T.; Garcia, J.-L.; Coker, A.; Bugg, T.D.H.; Wood, S.P.
Deposited on	:	2004-07-19
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

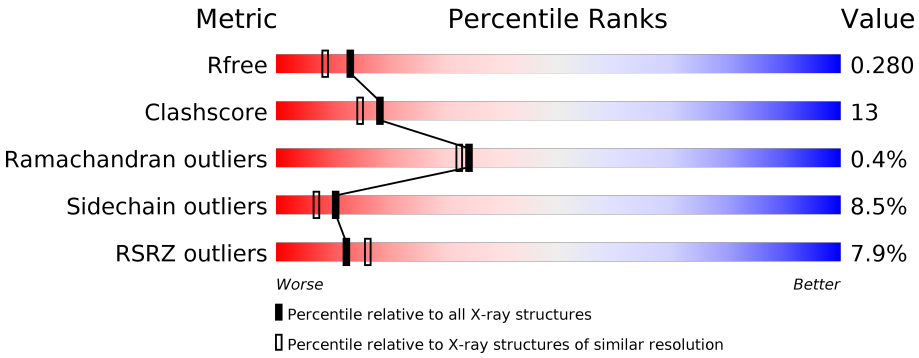
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	289	9% 71% 25%
1	B	289	9% 69% 28%
1	C	289	6% 73% 24%
1	D	289	8% 71% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9492 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 2-hydroxy-6-ketonona-2,4-dienedioic acid hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	19	1	0
			2244	1419	402	412	11			
1	B	286	Total	C	N	O	S	124	1	0
			2244	1419	402	412	11			
1	C	286	Total	C	N	O	S	30	0	0
			2234	1413	399	411	11			
1	D	285	Total	C	N	O	S	23	0	0
			2222	1404	398	409	11			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

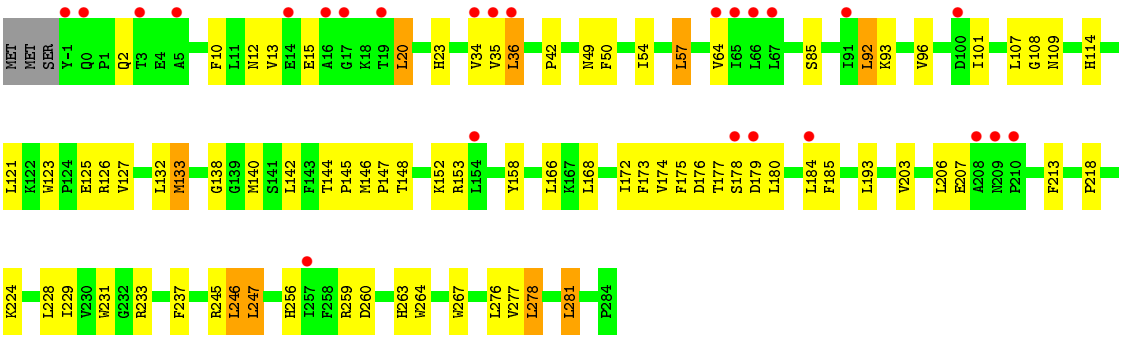
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	106	Total	O	0	0
			106	106		
3	C	158	Total	O	0	0
			158	158		
3	D	153	Total	O	0	0
			153	153		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

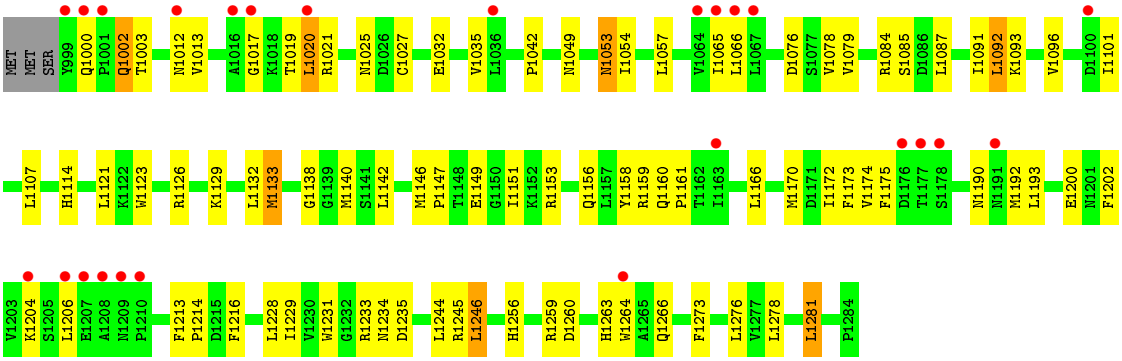
- Molecule 1: 2-hydroxy-6-ketonona-2,4-dienedioic acid hydrolase

Chain A:



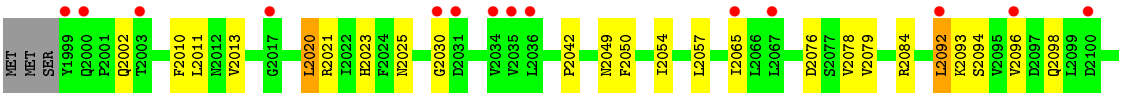
- Molecule 1: 2-hydroxy-6-ketonona-2,4-dienedioic acid hydrolase

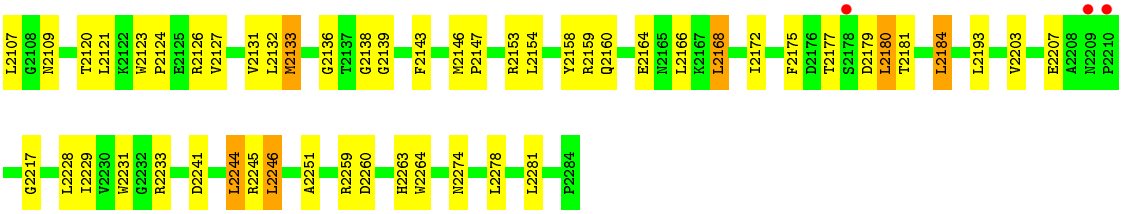
Chain B:



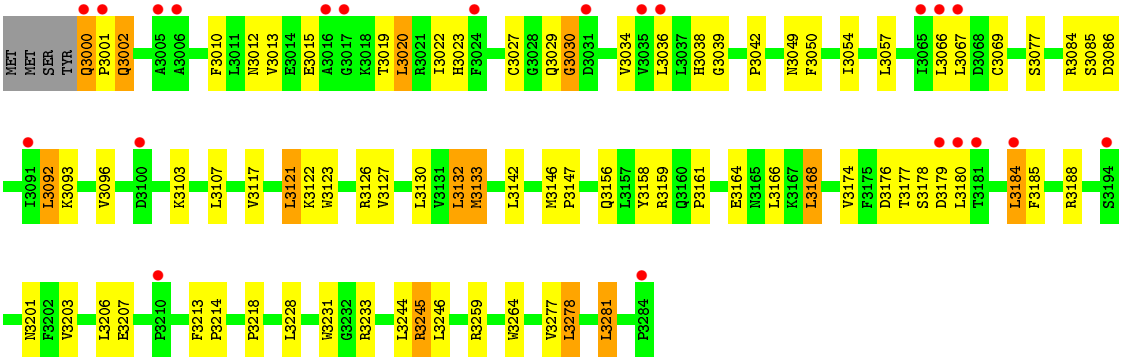
- Molecule 1: 2-hydroxy-6-ketonona-2,4-dienedioic acid hydrolase

Chain C:





• Molecule 1: 2-hydroxy-6-ketonona-2,4-dienedioic acid hydrolase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.86Å 144.15Å 62.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-2.10) 93.2 (19.91-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.278 0.221 , 0.280	Depositor DCC
R_{free} test set	3619 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 67.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9492	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.49% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.32	0/2295	0.60	0/3106
1	B	0.32	0/2295	0.59	0/3106
1	C	0.33	0/2284	0.61	0/3091
1	D	0.34	0/2271	0.60	0/3073
All	All	0.33	0/9145	0.60	0/12376

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	2244	0	2216	69	0
1	B	2244	0	2213	58	0
1	C	2234	0	2207	53	0
1	D	2222	0	2198	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	127	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	106	0	0	3	0
3	C	158	0	0	0	0
3	D	153	0	0	3	0
All	All	9492	0	8834	230	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 (230) 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:245:ARG:HG2	1:D:3142:LEU:HD21	1.58	0.84
1:A:20:LEU:HD23	1:A:20:LEU:H	1.43	0.82
1:D:3233:ARG:HH11	1:D:3233:ARG:HG3	1.45	0.81
1:B:1096:VAL:HG12	1:B:1126:ARG:NH2	1.98	0.79
1:D:3013:VAL:O	1:D:3020:LEU:HD23	1.83	0.77
1:D:3038:HIS:HE1	1:D:3069:CYS:H	1.28	0.76
1:A:203:VAL:O	1:A:207:GLU:HG3	1.91	0.69
1:B:1093:LYS:HG3	1:B:1123:TRP:CZ2	2.29	0.68
1:C:2120:THR:HG23	1:C:2127:VAL:HG21	1.75	0.68
1:A:142:LEU:HD21	1:D:3245:ARG:HG2	1.75	0.67
1:C:2020:LEU:HD23	1:C:2020:LEU:H	1.60	0.66
1:D:3020:LEU:HD23	1:D:3020:LEU:H	1.58	0.66
1:A:233:ARG:HH11	1:A:233:ARG:HG3	1.60	0.66
1:C:2274:ASN:O	1:C:2278:LEU:HD13	1.96	0.65
1:D:3085:SER:HG	1:D:3213:PHE:HD2	1.43	0.65
1:B:1142:LEU:HD21	1:C:2245:ARG:HG2	1.78	0.65
1:D:3233:ARG:HG3	1:D:3233:ARG:NH1	2.11	0.64
1:A:96:VAL:HG12	1:A:126:ARG:NH2	2.13	0.64
1:D:3180:LEU:HD22	1:D:3180:LEU:H	1.62	0.64
1:D:3010:PHE:CE1	1:D:3023:HIS:HB2	2.33	0.63
1:C:2042:PRO:HG3	1:C:2158:TYR:CE2	2.33	0.63
1:D:3233:ARG:HB3	1:D:3259:ARG:HA	1.80	0.63
1:C:2233:ARG:HB3	1:C:2259:ARG:HA	1.81	0.62
1:C:2013:VAL:O	1:C:2020:LEU:HD23	2.00	0.62
1:C:2021:ARG:N	1:C:2076:ASP:OD2	2.30	0.62
1:B:1053:ASN:O	1:B:1057:LEU:HD23	2.00	0.62
1:A:13:VAL:O	1:A:20:LEU:HD23	1.99	0.62
1:D:3000:GLN:OE1	1:D:3001:PRO:HD2	2.00	0.62
1:D:3015:GLU:HB3	1:D:3020:LEU:HD21	1.81	0.61
1:B:1202:PHE:O	1:B:1206:LEU:HD13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2177:THR:HA	1:C:2180:LEU:HD22	1.82	0.61
1:C:2203:VAL:O	1:C:2207:GLU:HG3	2.01	0.61
1:A:175:PHE:CE2	1:A:260:ASP:HB3	2.36	0.61
1:D:3166:LEU:HD22	1:D:3185:PHE:CZ	2.38	0.59
1:B:1133:MET:HB2	3:B:528:HOH:O	2.03	0.58
1:C:2146:MET:HA	1:C:2147:PRO:C	2.23	0.58
1:B:1138:GLY:O	1:B:1245:ARG:NH2	2.37	0.58
1:D:3038:HIS:HD2	1:D:3039:GLY:O	1.86	0.58
1:A:179:ASP:HB3	1:A:267:TRP:CZ3	2.39	0.57
1:A:93:LYS:HG3	1:A:123:TRP:CZ2	2.38	0.57
1:B:1020:LEU:HD23	1:B:1020:LEU:H	1.70	0.57
1:C:2159:ARG:HB2	1:C:2159:ARG:HH11	1.69	0.57
1:B:1042:PRO:HG3	1:B:1158:TYR:CE2	2.40	0.56
1:A:20:LEU:N	1:A:20:LEU:HD23	2.17	0.56
1:D:3184:LEU:HD11	1:D:3264:TRP:CZ3	2.40	0.56
1:A:233:ARG:NH1	1:A:233:ARG:HG3	2.21	0.56
1:D:3146:MET:HA	1:D:3147:PRO:C	2.25	0.56
1:B:1093:LYS:HG3	1:B:1123:TRP:CH2	2.41	0.55
1:D:3203:VAL:O	1:D:3207:GLU:HG3	2.06	0.55
1:C:2154:LEU:HD23	1:C:2154:LEU:C	2.26	0.55
1:C:2241:ASP:HA	1:C:2244:LEU:HD22	1.88	0.55
1:D:3038:HIS:CE1	1:D:3069:CYS:H	2.18	0.55
1:A:93:LYS:HG3	1:A:123:TRP:CH2	2.42	0.55
1:A:42:PRO:HG3	1:A:158:TYR:CE2	2.41	0.55
1:B:1042:PRO:HG3	1:B:1158:TYR:CD2	2.42	0.54
1:D:3002:GLN:HG2	1:D:3027:CYS:HB3	1.88	0.54
1:A:184:LEU:HD11	1:A:264:TRP:CZ3	2.42	0.54
1:B:1235:ASP:OD2	1:B:1263:HIS:HD2	1.90	0.54
1:D:3092:LEU:O	1:D:3096:VAL:HG22	2.08	0.54
1:A:180:LEU:HD22	1:A:180:LEU:H	1.71	0.54
1:B:1087:LEU:O	1:B:1091:ILE:HG12	2.08	0.54
1:C:2011:LEU:HG	1:C:2098:GLN:OE1	2.07	0.54
1:A:10:PHE:CE1	1:A:23:HIS:HB2	2.43	0.53
1:A:229:ILE:HD13	1:A:246:LEU:HB3	1.91	0.53
1:A:35:VAL:HG11	1:A:92:LEU:HD11	1.89	0.53
1:B:1035:VAL:HG11	1:B:1092:LEU:HD11	1.91	0.53
1:B:1021:ARG:N	1:B:1076:ASP:OD2	2.33	0.53
1:A:34:VAL:HG12	1:A:36:LEU:CD1	2.39	0.53
1:A:114[B]:HIS:NE2	1:A:213:PHE:HB3	2.24	0.52
1:B:1233:ARG:HB3	1:B:1259:ARG:HA	1.90	0.52
1:D:3277:VAL:HG12	1:D:3281:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:HB3	1:A:20:LEU:HD21	1.90	0.51
1:C:2050:PHE:O	1:C:2054:ILE:HG13	2.10	0.51
1:C:2107:LEU:HD12	1:C:2131:VAL:HB	1.92	0.51
1:A:114[B]:HIS:CD2	1:A:213:PHE:HB3	2.44	0.51
1:B:1173:PHE:HD2	1:B:1174:VAL:HG13	1.75	0.51
1:D:3164:GLU:OE1	1:D:3164:GLU:HA	2.11	0.51
1:D:3176:ASP:OD1	1:D:3178:SER:HB3	2.11	0.51
1:D:3166:LEU:C	1:D:3166:LEU:HD23	2.31	0.51
1:A:20:LEU:N	1:A:20:LEU:CD2	2.74	0.51
1:D:3020:LEU:N	1:D:3020:LEU:HD23	2.26	0.51
1:A:166:LEU:HD23	1:A:166:LEU:O	2.11	0.51
1:B:1200:GLU:O	1:B:1204:LYS:HG3	2.11	0.51
1:B:1013:VAL:O	1:B:1020:LEU:HD23	2.11	0.50
1:B:1114[B]:HIS:CD2	1:B:1213:PHE:HB3	2.46	0.50
1:D:3085:SER:OG	1:D:3213:PHE:HD2	1.93	0.50
1:B:1153:ARG:HD2	1:B:1172:ILE:CD1	2.42	0.50
1:D:3042:PRO:HG3	1:D:3158:TYR:CE2	2.47	0.50
1:C:2159:ARG:HB2	1:C:2159:ARG:NH1	2.26	0.50
1:D:3184:LEU:HD11	1:D:3264:TRP:HZ3	1.75	0.50
1:C:2164:GLU:O	1:C:2168:LEU:HD22	2.11	0.50
1:D:3022:ILE:HG21	1:D:3067:LEU:HD11	1.94	0.50
1:D:3107:LEU:C	1:D:3133:MET:HE2	2.32	0.49
1:A:125:GLU:H	1:A:125:GLU:CD	2.15	0.49
1:B:1093:LYS:HG3	1:B:1123:TRP:CE2	2.46	0.49
1:C:2010:PHE:CE1	1:C:2023:HIS:HB2	2.48	0.49
1:C:2233:ARG:HH11	1:C:2233:ARG:HG3	1.77	0.49
1:D:3086:ASP:OD2	1:D:3122:LYS:HE3	2.13	0.49
1:A:146:MET:HA	1:A:147:PRO:C	2.33	0.49
1:A:184:LEU:C	1:A:184:LEU:HD23	2.34	0.49
1:C:2078:VAL:HG22	1:C:2079:VAL:N	2.28	0.49
1:A:42:PRO:HG3	1:A:158:TYR:CD2	2.48	0.49
1:C:2092:LEU:HD22	1:C:2096:VAL:HG23	1.93	0.48
1:D:3012:ASN:HD22	1:D:3019:THR:CG2	2.26	0.48
1:A:177:THR:HA	1:A:180:LEU:CD2	2.43	0.48
1:A:20:LEU:CD2	1:A:20:LEU:H	2.17	0.48
1:A:277:VAL:HG12	1:A:281:LEU:HD22	1.95	0.48
1:B:1193:LEU:HD22	1:B:1193:LEU:H	1.79	0.48
1:B:1235:ASP:OD2	1:B:1263:HIS:CD2	2.66	0.48
1:D:3015:GLU:HB3	1:D:3020:LEU:CD2	2.44	0.47
1:A:93:LYS:HG3	1:A:123:TRP:CE2	2.50	0.47
1:C:2096:VAL:HG12	1:C:2126:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2042:PRO:HG3	1:C:2158:TYR:CD2	2.49	0.47
1:B:1096:VAL:HG13	1:B:1101:ILE:HB	1.96	0.47
1:B:1096:VAL:CG1	1:B:1126:ARG:NH2	2.76	0.47
1:D:3177:THR:HA	1:D:3180:LEU:CD2	2.44	0.47
1:B:1153:ARG:HD2	1:B:1172:ILE:HD11	1.95	0.47
1:C:2020:LEU:HD23	1:C:2020:LEU:N	2.28	0.47
1:C:2184:LEU:HD11	1:C:2264:TRP:HZ3	1.80	0.47
1:C:2138:GLY:O	1:C:2245:ARG:NH2	2.48	0.47
1:B:1012:ASN:HD22	1:B:1019:THR:CG2	2.28	0.47
1:B:1078:VAL:HG22	1:B:1079:VAL:N	2.30	0.47
1:B:1085:SER:HG	1:B:1114[B]:HIS:CE1	2.24	0.47
1:A:138:GLY:O	1:A:245:ARG:NH2	2.48	0.46
1:A:109:ASN:HA	1:A:133:MET:HG2	1.97	0.46
1:A:166:LEU:HD22	1:A:185:PHE:CE2	2.51	0.46
1:D:3206:LEU:HD11	3:D:534:HOH:O	2.16	0.46
1:B:1002:GLN:HG2	1:B:1027:CYS:HB3	1.98	0.46
1:C:2153:ARG:HD2	1:C:2172:ILE:CD1	2.46	0.46
1:A:144:THR:HA	1:A:145:PRO:HD3	1.86	0.46
1:B:1256:HIS:CD2	1:B:1276:LEU:HD11	2.50	0.46
1:A:173:PHE:HD1	1:A:237:PHE:CZ	2.33	0.46
1:A:174:VAL:CG2	1:A:180:LEU:HD21	2.46	0.46
1:A:224:LYS:HD2	3:A:1078:HOH:O	2.15	0.46
1:B:1229:ILE:CD1	1:B:1246:LEU:HB3	2.45	0.46
1:C:2124:PRO:O	1:C:2127:VAL:HG22	2.16	0.46
1:A:108:GLY:O	1:A:133:MET:HG2	2.15	0.45
1:A:57:LEU:HB3	1:A:64:VAL:HG21	1.97	0.45
1:D:3093:LYS:HG3	1:D:3123:TRP:CH2	2.51	0.45
1:A:15:GLU:HB3	1:A:20:LEU:CD2	2.46	0.45
1:D:3166:LEU:O	1:D:3166:LEU:HD23	2.15	0.45
1:A:96:VAL:HG13	1:A:101:ILE:HB	1.97	0.45
1:B:1146:MET:HA	1:B:1147:PRO:C	2.36	0.45
1:B:1160:GLN:HA	1:B:1160:GLN:HE21	1.81	0.45
1:B:1229:ILE:HD13	1:B:1246:LEU:HB3	1.98	0.45
1:D:3050:PHE:O	1:D:3054:ILE:HG13	2.17	0.45
1:A:184:LEU:HD11	1:A:264:TRP:HZ3	1.81	0.45
1:C:2042:PRO:HG3	1:C:2158:TYR:CZ	2.51	0.45
1:A:50:PHE:O	1:A:54:ILE:HG13	2.17	0.45
1:B:1233:ARG:HG3	1:B:1234:ASN:HD22	1.81	0.45
1:D:3000:GLN:HA	1:D:3001:PRO:HD2	1.86	0.45
1:A:193:LEU:H	1:A:193:LEU:HD22	1.82	0.45
1:C:2177:THR:HA	1:C:2180:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3103:LYS:NZ	3:D:108:HOH:O	2.49	0.44
1:D:3177:THR:C	1:D:3179:ASP:H	2.21	0.44
1:B:1114[B]:HIS:CE1	1:B:1216:PHE:CE2	3.05	0.44
1:D:3038:HIS:HE1	1:D:3069:CYS:N	2.05	0.44
1:A:247:LEU:O	1:C:2259:ARG:HD2	2.17	0.44
1:A:278:LEU:HA	1:A:278:LEU:HD12	1.84	0.44
1:C:2160:GLN:HA	1:C:2160:GLN:NE2	2.33	0.44
1:D:3042:PRO:HG3	1:D:3158:TYR:CD2	2.52	0.44
1:A:36:LEU:HD12	1:A:107:LEU:HB2	2.00	0.44
1:C:2175:PHE:CE2	1:C:2260:ASP:HB3	2.53	0.44
1:A:85:SER:HG	1:A:114[B]:HIS:CE1	2.29	0.43
1:D:3066:LEU:N	1:D:3066:LEU:HD12	2.32	0.43
1:D:3130:LEU:HG	1:D:3132:LEU:HD13	2.00	0.43
1:A:256:HIS:CG	1:A:276:LEU:HD11	2.53	0.43
1:D:3103:LYS:HA	1:D:3126:ARG:O	2.18	0.43
1:A:148:THR:O	1:A:152:LYS:HG3	2.19	0.43
1:C:2143:PHE:HB3	3:D:156:HOH:O	2.17	0.43
1:C:2153:ARG:HD2	1:C:2172:ILE:HD11	2.00	0.43
1:C:2136:GLY:HA3	1:C:2246:LEU:HD21	2.01	0.43
1:A:233:ARG:HB3	1:A:259:ARG:HA	1.99	0.43
1:B:1149:GLU:HG2	1:B:1172:ILE:HD12	2.01	0.43
1:B:1166:LEU:HD12	1:B:1192:MET:SD	2.59	0.43
1:B:1175:PHE:CE2	1:B:1260:ASP:HB3	2.53	0.43
1:A:175:PHE:CD2	1:A:260:ASP:HB3	2.54	0.43
1:B:1025:ASN:O	1:B:1065:ILE:HA	2.19	0.43
1:C:2013:VAL:HG13	1:C:2094:SER:CB	2.49	0.43
1:C:2020:LEU:N	1:C:2020:LEU:CD2	2.82	0.43
1:D:3117:VAL:HG12	1:D:3121:LEU:HD22	2.01	0.43
1:D:3213:PHE:HA	1:D:3214:PRO:HD3	1.87	0.43
1:C:2263:HIS:O	1:C:2263:HIS:CG	2.72	0.43
1:B:1085:SER:OG	1:B:1213:PHE:HD1	2.01	0.43
1:A:176:ASP:OD1	1:A:178:SER:HB2	2.18	0.43
1:B:1166:LEU:O	1:B:1170:MET:HG2	2.19	0.43
1:A:153:ARG:HD2	1:A:172:ILE:HD11	2.01	0.43
1:B:1002:GLN:HE21	1:B:1002:GLN:CA	2.31	0.43
1:C:2139:GLY:HA3	1:C:2245:ARG:NH2	2.34	0.42
1:C:2159:ARG:CB	1:C:2159:ARG:HH11	2.31	0.42
1:C:2109:ASN:HA	1:C:2133:MET:HG2	2.01	0.42
1:B:1085:SER:HG	1:B:1114[B]:HIS:CG	2.29	0.42
1:C:2025:ASN:O	1:C:2065:ILE:HA	2.19	0.42
1:D:3156:GLN:CD	1:D:3159:ARG:HH12	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD22	1:C:2259:ARG:HB2	2.01	0.42
1:C:2241:ASP:HA	1:C:2244:LEU:CD2	2.49	0.42
1:A:12:ASN:N	1:A:12:ASN:HD22	2.16	0.42
1:B:1173:PHE:CD2	1:B:1174:VAL:HG13	2.53	0.42
1:B:1020:LEU:CD2	1:B:1020:LEU:H	2.32	0.42
1:A:193:LEU:N	1:A:193:LEU:HD22	2.34	0.42
1:A:174:VAL:HG21	1:A:180:LEU:HD21	2.01	0.42
1:B:1173:PHE:CE2	1:B:1264:TRP:HB2	2.55	0.42
1:B:1264:TRP:CD1	1:B:1266:GLN:HG2	2.55	0.42
1:C:2233:ARG:HG3	1:C:2233:ARG:NH1	2.34	0.42
1:A:123:TRP:HA	1:A:125:GLU:OE2	2.19	0.42
1:B:1156:GLN:HA	1:B:1159:ARG:NH1	2.35	0.41
3:B:263:HOH:O	1:C:2217:GLY:HA3	2.19	0.41
1:A:259:ARG:HD3	1:C:2251:ALA:HA	2.03	0.41
1:A:179:ASP:C	1:A:267:TRP:HH2	2.24	0.41
1:D:3034:VAL:HG12	1:D:3036:LEU:CD1	2.51	0.41
1:D:3168:LEU:HA	1:D:3168:LEU:HD12	1.92	0.41
1:B:1133:MET:HE1	1:B:1273:PHE:HZ	1.85	0.41
1:B:1213:PHE:HA	1:B:1214:PRO:HD3	1.92	0.41
1:C:2093:LYS:HG3	1:C:2123:TRP:CZ2	2.55	0.41
1:C:2229:ILE:HD13	1:C:2246:LEU:HB3	2.01	0.41
1:C:2181:THR:OG1	1:C:2184:LEU:HB2	2.21	0.41
1:A:263:HIS:CG	1:A:263:HIS:O	2.74	0.41
1:D:3174:VAL:CG2	1:D:3180:LEU:HD21	2.51	0.41
1:B:1129:LYS:HD2	1:B:1281:LEU:HA	2.02	0.41
1:B:1160:GLN:HA	1:B:1160:GLN:NE2	2.36	0.41
1:A:245:ARG:HA	1:D:3142:LEU:CD2	2.51	0.41
1:A:218:PRO:HG2	1:D:3218:PRO:HG2	2.02	0.41
1:B:1054:ILE:HD11	1:B:1066:LEU:HD21	2.02	0.40
1:D:3029:GLN:O	1:D:3030:GLY:O	2.39	0.40
1:D:3077:SER:OG	1:D:3201:ASN:ND2	2.47	0.40
1:A:92:LEU:HD22	1:A:96:VAL:HG23	2.03	0.40
1:B:1003:THR:HB	3:B:438:HOH:O	2.20	0.40
1:B:1020:LEU:N	1:B:1020:LEU:CD2	2.85	0.40
1:A:179:ASP:CB	1:A:267:TRP:CZ3	3.04	0.40
1:D:3278:LEU:HA	1:D:3278:LEU:HD12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	285/289 (99%)	276 (97%)	9 (3%)	0	100	100
1	B	285/289 (99%)	269 (94%)	14 (5%)	2 (1%)	22	18
1	C	284/289 (98%)	273 (96%)	10 (4%)	1 (0%)	34	32
1	D	283/289 (98%)	267 (94%)	14 (5%)	2 (1%)	22	18
All	All	1137/1156 (98%)	1085 (95%)	47 (4%)	5 (0%)	34	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2030	GLY
1	D	3030	GLY
1	B	1017	GLY
1	B	1161	PRO
1	D	3161	PRO

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	240/242 (99%)	221 (92%)	19 (8%)	12	9
1	B	240/242 (99%)	219 (91%)	21 (9%)	10	6
1	C	239/242 (99%)	219 (92%)	20 (8%)	11	7
1	D	238/242 (98%)	217 (91%)	21 (9%)	10	6
All	All	957/968 (99%)	876 (92%)	81 (8%)	10	7

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	20	LEU
1	A	36	LEU
1	A	49	ASN
1	A	57	LEU
1	A	92	LEU
1	A	121	LEU
1	A	127	VAL
1	A	132	LEU
1	A	133	MET
1	A	140	MET
1	A	168	LEU
1	A	206	LEU
1	A	228	LEU
1	A	231	TRP
1	A	246	LEU
1	A	247	LEU
1	A	278	LEU
1	A	281	LEU
1	B	1000	GLN
1	B	1002	GLN
1	B	1020	LEU
1	B	1032	GLU
1	B	1049	ASN
1	B	1053	ASN
1	B	1084	ARG
1	B	1092	LEU
1	B	1107	LEU
1	B	1121	LEU
1	B	1132	LEU
1	B	1133	MET
1	B	1140	MET
1	B	1151	ILE
1	B	1190	ASN
1	B	1228	LEU
1	B	1231	TRP
1	B	1244	LEU
1	B	1246	LEU
1	B	1278	LEU
1	B	1281	LEU
1	C	2002	GLN
1	C	2020	LEU

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Mol	Chain	Res	Type
1	C	2049	ASN
1	C	2057	LEU
1	C	2084	ARG
1	C	2092	LEU
1	C	2121	LEU
1	C	2132	LEU
1	C	2133	MET
1	C	2166	LEU
1	C	2168	LEU
1	C	2179	ASP
1	C	2180	LEU
1	C	2184	LEU
1	C	2193	LEU
1	C	2228	LEU
1	C	2231	TRP
1	C	2244	LEU
1	C	2246	LEU
1	C	2281	LEU
1	D	3000	GLN
1	D	3002	GLN
1	D	3020	LEU
1	D	3049	ASN
1	D	3057	LEU
1	D	3084	ARG
1	D	3092	LEU
1	D	3121	LEU
1	D	3127	VAL
1	D	3132	LEU
1	D	3133	MET
1	D	3168	LEU
1	D	3184	LEU
1	D	3188	ARG
1	D	3228	LEU
1	D	3231	TRP
1	D	3244	LEU
1	D	3245	ARG
1	D	3246	LEU
1	D	3278	LEU
1	D	3281	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	12	ASN
1	A	109	ASN
1	A	155	ASN
1	A	160	GLN
1	B	1000	GLN
1	B	1002	GLN
1	B	1012	ASN
1	B	1109	ASN
1	B	1155	ASN
1	B	1160	GLN
1	B	1234	ASN
1	B	1263	HIS
1	C	2000	GLN
1	C	2002	GLN
1	C	2160	GLN
1	C	2226	GLN
1	D	3002	GLN
1	D	3012	ASN
1	D	3038	HIS
1	D	3160	GLN
1	D	3191	ASN
1	D	3201	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 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	286/289 (98%)	0.36	25 (8%)	10	13	20, 35, 51, 62	5 (1%)
1	B	274/289 (94%)	0.49	25 (9%)	9	12	20, 39, 56, 62	7 (2%)
1	C	286/289 (98%)	0.24	17 (5%)	22	27	19, 34, 51, 63	8 (2%)
1	D	285/289 (98%)	0.34	22 (7%)	13	17	19, 34, 52, 65	6 (2%)
All	All	1131/1156 (97%)	0.36	89 (7%)	12	16	19, 36, 53, 65	26 (2%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1017	GLY	5.9
1	C	1999	TYR	5.2
1	B	999	TYR	4.5
1	A	-1	TYR	4.5
1	B	1000	GLN	4.4
1	B	1016	ALA	4.4
1	D	3016	ALA	4.4
1	D	3066	LEU	4.4
1	B	1177	THR	4.2
1	C	2100	ASP	4.0
1	A	66	LEU	3.8
1	C	2000	GLN	3.8
1	C	2031	ASP	3.8
1	A	36	LEU	3.7
1	B	1065	ILE	3.7
1	B	1163	ILE	3.6
1	A	17	GLY	3.6
1	A	5	ALA	3.6
1	A	179	ASP	3.6
1	B	1001	PRO	3.6
1	C	2178	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	3179	ASP	3.5
1	D	3000	GLN	3.5
1	D	3100	ASP	3.5
1	B	1207	GLU	3.5
1	B	1100	ASP	3.4
1	B	1020	LEU	3.4
1	B	1066	LEU	3.3
1	D	3035	VAL	3.3
1	C	2017	GLY	3.3
1	B	1064	VAL	3.3
1	B	1191	ASN	3.3
1	C	2035	VAL	3.3
1	C	2067	LEU	3.3
1	A	65	ILE	3.2
1	A	178	SER	3.2
1	D	3031	ASP	3.2
1	B	1208	ALA	3.1
1	D	3065	ILE	3.1
1	D	3001	PRO	3.1
1	A	67	LEU	3.0
1	A	35	VAL	2.9
1	A	14	GLU	2.9
1	C	2030	GLY	2.9
1	A	0	GLN	2.9
1	B	1206	LEU	2.9
1	D	3036	LEU	2.8
1	D	3284	PRO	2.8
1	D	3017	GLY	2.8
1	A	209	ASN	2.7
1	D	3067	LEU	2.7
1	A	64	VAL	2.7
1	C	2209	ASN	2.6
1	D	3005	ALA	2.6
1	B	1067	LEU	2.6
1	B	1178	SER	2.5
1	A	257	ILE	2.5
1	A	34	VAL	2.5
1	C	2065	ILE	2.4
1	D	3006	ALA	2.4
1	B	1209	ASN	2.4
1	B	1210	PRO	2.4
1	D	3181	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	3091	ILE	2.4
1	A	154	LEU	2.4
1	D	3180	LEU	2.3
1	B	1012	ASN	2.3
1	B	1264	TRP	2.3
1	C	2034	VAL	2.3
1	B	1176	ASP	2.3
1	A	184	LEU	2.2
1	C	2210	PRO	2.2
1	C	2096	VAL	2.2
1	C	2092	LEU	2.2
1	D	3184	LEU	2.1
1	A	100	ASP	2.1
1	B	1204	LYS	2.1
1	A	3	THR	2.1
1	A	16	ALA	2.1
1	A	208	ALA	2.1
1	A	91	ILE	2.1
1	A	19	THR	2.1
1	D	3024	PHE	2.1
1	C	2036	LEU	2.0
1	D	3210	PRO	2.0
1	D	3194	SER	2.0
1	A	210	PRO	2.0
1	B	1036	LEU	2.0
1	C	2003	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	B	1285	1/1	0.95	0.11	47,47,47,47	0
2	CL	A	1002	1/1	0.98	0.15	41,41,41,41	0
2	CL	C	1003	1/1	0.98	0.14	36,36,36,36	0
2	CL	D	1001	1/1	0.99	0.13	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.