WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 06:28 PM EDT

PDB ID	:	4IL0
Title	:	Crystal structure of GlucDRP from E. coli K-12 MG1655 (EFI target EFI-506058)
Authors	:	Lukk, T.; Ghasempur, S.; Imker, H.J.; Gerlt, J.A.; Nair, S.K.; Enzyme Function Initiative (EFI)
Deposited on	:	2012-12-28
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

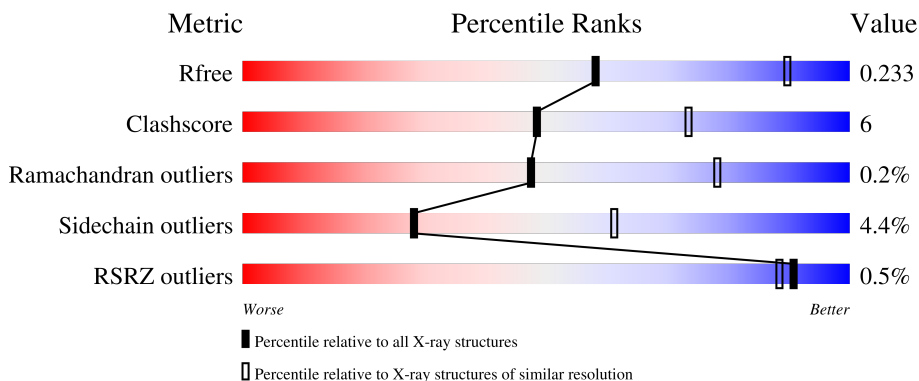|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		4.4%
RSRZ outliers		0.5%

Worse ——— *Better*

▮ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	466	77% · 17% · 6%
1	B	466	80% · 13% · 6%
1	C	466	77% · 17% · 6%
1	D	466	76% · 15% · 9%
1	E	466	78% · 11% · 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	466	78%　　　　　　　　　　　　　　　15%　　・　6%
1	G	466	76%　　　　　　　　　　　　　　　12%　　・　11%
1	H	466	.%　75%　　　　　　　　　　　　　　15%　　・　9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	C	501	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27172 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 Glucarate dehydratase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3396	2153	601	626	16			
1	B	440	Total	C	N	O	S	0	0	0
			3396	2153	601	626	16			
1	C	440	Total	C	N	O	S	0	0	0
			3396	2153	601	626	16			
1	D	424	Total	C	N	O	S	0	0	0
			3275	2076	580	603	16			
1	E	417	Total	C	N	O	S	0	0	0
			3224	2045	570	593	16			
1	F	439	Total	C	N	O	S	0	0	0
			3390	2150	600	624	16			
1	G	416	Total	C	N	O	S	0	0	0
			3215	2039	569	591	16			
1	H	426	Total	C	N	O	S	0	0	0
			3283	2082	583	602	16			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q46915
A	-18	GLY	-	expression tag	UNP Q46915
A	-17	SER	-	expression tag	UNP Q46915
A	-16	SER	-	expression tag	UNP Q46915
A	-15	HIS	-	expression tag	UNP Q46915
A	-14	HIS	-	expression tag	UNP Q46915
A	-13	HIS	-	expression tag	UNP Q46915
A	-12	HIS	-	expression tag	UNP Q46915
A	-11	HIS	-	expression tag	UNP Q46915
A	-10	HIS	-	expression tag	UNP Q46915
A	-9	SER	-	expression tag	UNP Q46915
A	-8	SER	-	expression tag	UNP Q46915
A	-7	GLY	-	expression tag	UNP Q46915

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q46915
A	-5	VAL	-	expression tag	UNP Q46915
A	-4	PRO	-	expression tag	UNP Q46915
A	-3	ARG	-	expression tag	UNP Q46915
A	-2	GLY	-	expression tag	UNP Q46915
A	-1	SER	-	expression tag	UNP Q46915
A	0	HIS	-	expression tag	UNP Q46915
B	-19	MET	-	expression tag	UNP Q46915
B	-18	GLY	-	expression tag	UNP Q46915
B	-17	SER	-	expression tag	UNP Q46915
B	-16	SER	-	expression tag	UNP Q46915
B	-15	HIS	-	expression tag	UNP Q46915
B	-14	HIS	-	expression tag	UNP Q46915
B	-13	HIS	-	expression tag	UNP Q46915
B	-12	HIS	-	expression tag	UNP Q46915
B	-11	HIS	-	expression tag	UNP Q46915
B	-10	HIS	-	expression tag	UNP Q46915
B	-9	SER	-	expression tag	UNP Q46915
B	-8	SER	-	expression tag	UNP Q46915
B	-7	GLY	-	expression tag	UNP Q46915
B	-6	LEU	-	expression tag	UNP Q46915
B	-5	VAL	-	expression tag	UNP Q46915
B	-4	PRO	-	expression tag	UNP Q46915
B	-3	ARG	-	expression tag	UNP Q46915
B	-2	GLY	-	expression tag	UNP Q46915
B	-1	SER	-	expression tag	UNP Q46915
B	0	HIS	-	expression tag	UNP Q46915
C	-19	MET	-	expression tag	UNP Q46915
C	-18	GLY	-	expression tag	UNP Q46915
C	-17	SER	-	expression tag	UNP Q46915
C	-16	SER	-	expression tag	UNP Q46915
C	-15	HIS	-	expression tag	UNP Q46915
C	-14	HIS	-	expression tag	UNP Q46915
C	-13	HIS	-	expression tag	UNP Q46915
C	-12	HIS	-	expression tag	UNP Q46915
C	-11	HIS	-	expression tag	UNP Q46915
C	-10	HIS	-	expression tag	UNP Q46915
C	-9	SER	-	expression tag	UNP Q46915
C	-8	SER	-	expression tag	UNP Q46915
C	-7	GLY	-	expression tag	UNP Q46915
C	-6	LEU	-	expression tag	UNP Q46915
C	-5	VAL	-	expression tag	UNP Q46915

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q46915
C	-3	ARG	-	expression tag	UNP Q46915
C	-2	GLY	-	expression tag	UNP Q46915
C	-1	SER	-	expression tag	UNP Q46915
C	0	HIS	-	expression tag	UNP Q46915
D	-19	MET	-	expression tag	UNP Q46915
D	-18	GLY	-	expression tag	UNP Q46915
D	-17	SER	-	expression tag	UNP Q46915
D	-16	SER	-	expression tag	UNP Q46915
D	-15	HIS	-	expression tag	UNP Q46915
D	-14	HIS	-	expression tag	UNP Q46915
D	-13	HIS	-	expression tag	UNP Q46915
D	-12	HIS	-	expression tag	UNP Q46915
D	-11	HIS	-	expression tag	UNP Q46915
D	-10	HIS	-	expression tag	UNP Q46915
D	-9	SER	-	expression tag	UNP Q46915
D	-8	SER	-	expression tag	UNP Q46915
D	-7	GLY	-	expression tag	UNP Q46915
D	-6	LEU	-	expression tag	UNP Q46915
D	-5	VAL	-	expression tag	UNP Q46915
D	-4	PRO	-	expression tag	UNP Q46915
D	-3	ARG	-	expression tag	UNP Q46915
D	-2	GLY	-	expression tag	UNP Q46915
D	-1	SER	-	expression tag	UNP Q46915
D	0	HIS	-	expression tag	UNP Q46915
E	-19	MET	-	expression tag	UNP Q46915
E	-18	GLY	-	expression tag	UNP Q46915
E	-17	SER	-	expression tag	UNP Q46915
E	-16	SER	-	expression tag	UNP Q46915
E	-15	HIS	-	expression tag	UNP Q46915
E	-14	HIS	-	expression tag	UNP Q46915
E	-13	HIS	-	expression tag	UNP Q46915
E	-12	HIS	-	expression tag	UNP Q46915
E	-11	HIS	-	expression tag	UNP Q46915
E	-10	HIS	-	expression tag	UNP Q46915
E	-9	SER	-	expression tag	UNP Q46915
E	-8	SER	-	expression tag	UNP Q46915
E	-7	GLY	-	expression tag	UNP Q46915
E	-6	LEU	-	expression tag	UNP Q46915
E	-5	VAL	-	expression tag	UNP Q46915
E	-4	PRO	-	expression tag	UNP Q46915
E	-3	ARG	-	expression tag	UNP Q46915

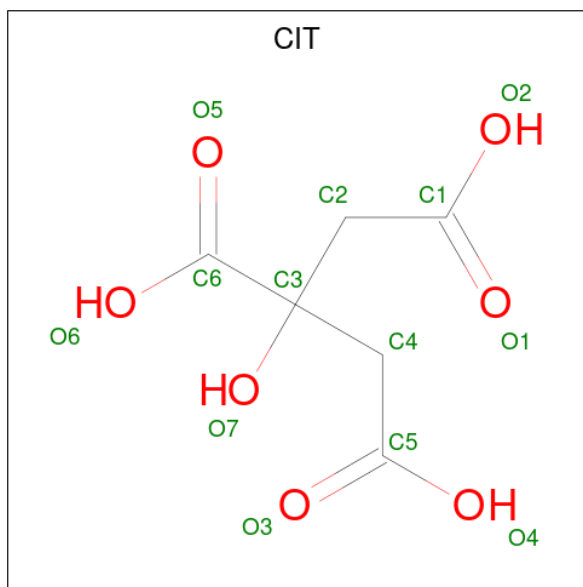*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q46915
E	-1	SER	-	expression tag	UNP Q46915
E	0	HIS	-	expression tag	UNP Q46915
F	-19	MET	-	expression tag	UNP Q46915
F	-18	GLY	-	expression tag	UNP Q46915
F	-17	SER	-	expression tag	UNP Q46915
F	-16	SER	-	expression tag	UNP Q46915
F	-15	HIS	-	expression tag	UNP Q46915
F	-14	HIS	-	expression tag	UNP Q46915
F	-13	HIS	-	expression tag	UNP Q46915
F	-12	HIS	-	expression tag	UNP Q46915
F	-11	HIS	-	expression tag	UNP Q46915
F	-10	HIS	-	expression tag	UNP Q46915
F	-9	SER	-	expression tag	UNP Q46915
F	-8	SER	-	expression tag	UNP Q46915
F	-7	GLY	-	expression tag	UNP Q46915
F	-6	LEU	-	expression tag	UNP Q46915
F	-5	VAL	-	expression tag	UNP Q46915
F	-4	PRO	-	expression tag	UNP Q46915
F	-3	ARG	-	expression tag	UNP Q46915
F	-2	GLY	-	expression tag	UNP Q46915
F	-1	SER	-	expression tag	UNP Q46915
F	0	HIS	-	expression tag	UNP Q46915
G	-19	MET	-	expression tag	UNP Q46915
G	-18	GLY	-	expression tag	UNP Q46915
G	-17	SER	-	expression tag	UNP Q46915
G	-16	SER	-	expression tag	UNP Q46915
G	-15	HIS	-	expression tag	UNP Q46915
G	-14	HIS	-	expression tag	UNP Q46915
G	-13	HIS	-	expression tag	UNP Q46915
G	-12	HIS	-	expression tag	UNP Q46915
G	-11	HIS	-	expression tag	UNP Q46915
G	-10	HIS	-	expression tag	UNP Q46915
G	-9	SER	-	expression tag	UNP Q46915
G	-8	SER	-	expression tag	UNP Q46915
G	-7	GLY	-	expression tag	UNP Q46915
G	-6	LEU	-	expression tag	UNP Q46915
G	-5	VAL	-	expression tag	UNP Q46915
G	-4	PRO	-	expression tag	UNP Q46915
G	-3	ARG	-	expression tag	UNP Q46915
G	-2	GLY	-	expression tag	UNP Q46915
G	-1	SER	-	expression tag	UNP Q46915

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q46915
H	-19	MET	-	expression tag	UNP Q46915
H	-18	GLY	-	expression tag	UNP Q46915
H	-17	SER	-	expression tag	UNP Q46915
H	-16	SER	-	expression tag	UNP Q46915
H	-15	HIS	-	expression tag	UNP Q46915
H	-14	HIS	-	expression tag	UNP Q46915
H	-13	HIS	-	expression tag	UNP Q46915
H	-12	HIS	-	expression tag	UNP Q46915
H	-11	HIS	-	expression tag	UNP Q46915
H	-10	HIS	-	expression tag	UNP Q46915
H	-9	SER	-	expression tag	UNP Q46915
H	-8	SER	-	expression tag	UNP Q46915
H	-7	GLY	-	expression tag	UNP Q46915
H	-6	LEU	-	expression tag	UNP Q46915
H	-5	VAL	-	expression tag	UNP Q46915
H	-4	PRO	-	expression tag	UNP Q46915
H	-3	ARG	-	expression tag	UNP Q46915
H	-2	GLY	-	expression tag	UNP Q46915
H	-1	SER	-	expression tag	UNP Q46915
H	0	HIS	-	expression tag	UNP Q46915

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 6	O 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 13	C 6	O 7	0	0
2	C	1	Total 13	C 6	O 7	0	0
2	D	1	Total 13	C 6	O 7	0	0
2	E	1	Total 13	C 6	O 7	0	0
2	F	1	Total 13	C 6	O 7	0	0
2	G	1	Total 13	C 6	O 7	0	0
2	H	1	Total 13	C 6	O 7	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
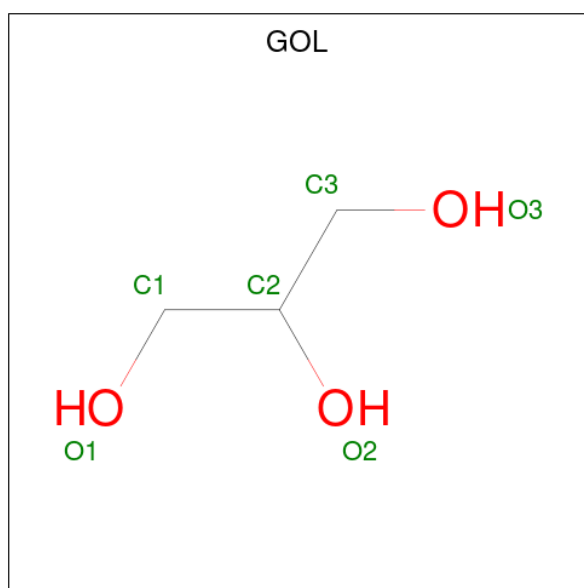
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total 71	O 71	0	0
4	B	74	Total 74	O 74	0	0
4	C	70	Total 70	O 70	0	0
4	D	68	Total 68	O 68	0	0
4	E	68	Total 68	O 68	0	0
4	F	59	Total 59	O 59	0	0
4	G	41	Total 41	O 41	0	0
4	H	30	Total 30	O 30	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 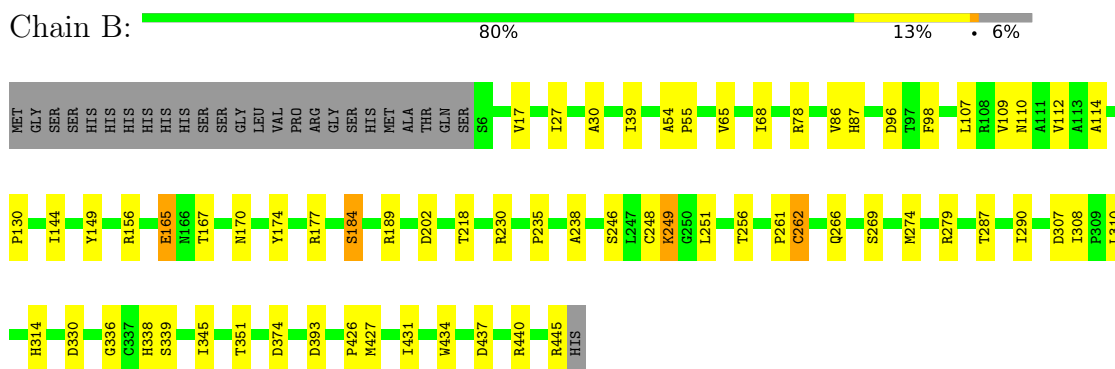view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron 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.
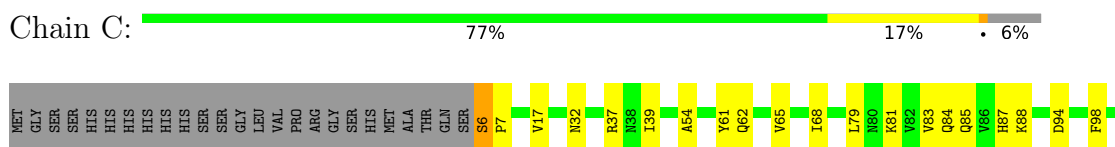
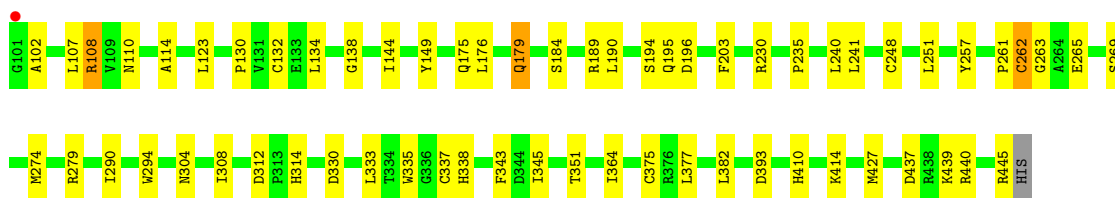• Molecule 1: Glucarate dehydratase-related protein

Chain A:

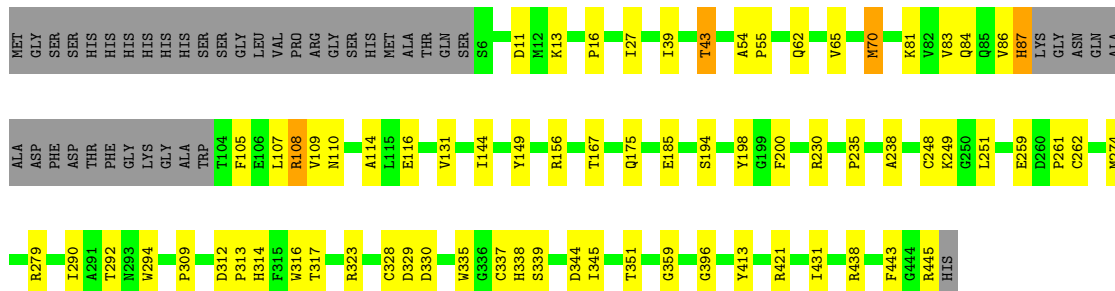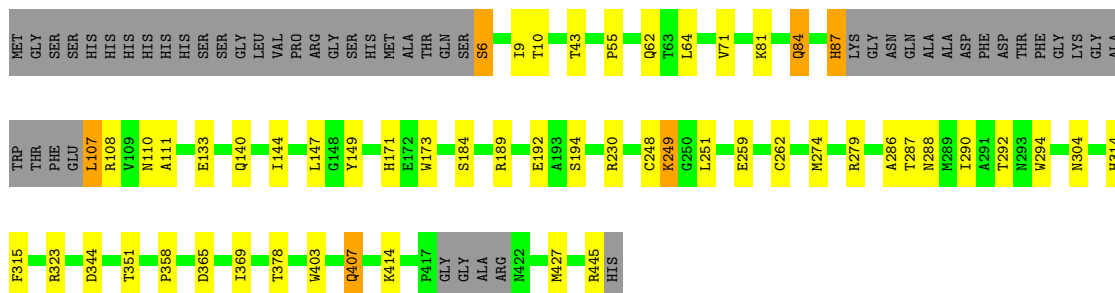
• Molecule 1: Glucarate dehydratase-related protein

Chain B:

• Molecule 1: Glucarate dehydratase-related protein

Chain C:

G101 A102 L107 R108 V109 N110 A114 L123 P130 V131 C132 E133 L134 G138 I144 Y149 Q175 L176 Q179 S184 R189 L190 S194 Q195 D196 F203 R230 P235 L240 L241 C248 L251 Y257 P261 C262 G263 A264 E265 S269

M274 R279 I290 W294 N304 I308 D312 P313 H314 D330 L333 T334 W335 G336 C337 H338 F343 D344 I345 T351 I364 C375 R376 L377 L382 D393 H410 K414 M427 D437 K438 R440 R445 HIS

• Molecule 1: Glucarate dehydratase-related protein

Chain D: 76% 15% 9%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA THR GLN SER S6 D11 M12 K13 P16 I27 I39 T43 A54 P55 Q62 V65 M70 K81 V82 V83 Q84 Q85 V86 H87 LYS GLY ASN GLN ALA

ALA ASP PHE ASP THR PHE GLY LYS GLY ALA TRP T104 F105 E106 L107 R108 V109 N110 A114 L115 E116 V131 I144 Y149 R156 T167 Q175 E185 S194 Y198 G199 F200 R230 P235 A238 C248 K249 G250 L251 E259 D260 P261 C262 M274

R279 I290 A291 T292 N293 W294 P309 D312 P313 H314 F315 W316 T317 R323 C328 D329 D330 W335 G336 C337 H338 S339 D344 I345 T351 G359 G396 Y413 R421 I431 R438 F443 G444 R445 HIS

• Molecule 1: Glucarate dehydratase-related protein

Chain E: 78% 11% 11%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA THR GLN SER S6 I9 T10 T43 P55 Q62 T63 L64 V71 K81 Q84 H87 LYS GLY ASN GLN ALA ASP PHE ASP THR PHE LYS GLY ALA

TRP THR PHE GLU L107 R108 V109 N110 A111 E133 Q140 I144 L147 G148 Y149 H171 E172 W173 S184 R189 E192 A193 S194 R230 C248 K249 G250 L251 E259 C262 M274 R279 A286 T287 N288 M289 I290 A291 T292 N293 W294 N304 H314

F315 R323 D344 T351 P358 D365 I369 T378 W403 Q407 K414 P417 GLY GLY ALA ARG N422 M427 R445 HIS

• Molecule 1: Glucarate dehydratase-related protein

Chain F: 78% 15% 6%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA THR GLN SER P7 V8 V17 G28 T43 D44 N45 A46 G47 A54 P55 Q62 V65 I68 V76 A77 R78 L79 V82 V83 Q84 Q85 V86 H87 K88

A93 D94 T97 G101 L107 R108 V109 N110 A114 L123 V131 L134 P137 I144 Y149 R156 T157 K158 K180 R189 Q195 F203 K224 R230 P235 L241 K249 P261 C262 E265 R271 M274 R278

V285 I290 N304 D307 D312 R323 D330 W335 G336 C337 H338 F343 T351 A355 T362 A363 I364 L377 L382 K388 V391 P392 L397 A409 M427 F436 D437 K438 R440 R445 HIS

• Molecule 1: Glucarate dehydratase-related protein

Chain G:

76%   12%   •   11%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS SER MET ALA THR GLN SER SER P7 T10 D11 V17 A18 G19 G28 Y34 T43 A54 I60 Y61 Q62 H87 LYS GLY ASN GLN ALA ALA ASP PHE ASP THR PHE GLY

LYS GLY ALA TRP PHE THR PHE GLU LEU ARG V109 A114 P130 Q140 I144 L147 G148 Y149 R156 T157 K158 T159 D160 L161 P168 W173 R177 K180 Q195 D196 R197 F200 R230 P235 C248 K249 G250 L251 P261 S269 M274 T287

N288 M289 I290 A291 T292 R323 D330 S339 N340 N341 H342 F343 D344 T351 D365 I369 D374 L377 D393 Q407 K408 A409 P417 GLY GLY A420 M427 Q428 Y429 W434 T435 F436 D437 R438 K439 R440 R445 HIS

• Molecule 1: Glucarate dehydratase-related protein

Chain H:

%

75%   15%   •   9%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS SER MET ALA THR GLN SER S6 I9 V17 M23 I27 T36 I39 A54 P55 G56 V65 I68 V71 V83 Q84 Q85 V86 H87 K88 D96 T97 F98

A102 N110 A114 L115 E116 V131 I144 Y149 G154 D155 R156 T157 LYS THR ASP LEU PRO TYR VAL GLU ASN THR PRO G169 N170 H171 E172 W173 Y174 E192 Y198 G208 R225 R230 V233 D234 P235 A238 L241 C248 L251 N252 P261

A264 E265 M274 R278 R279 L283 P284 V285 I290 N304 D312 P313 H314 F315 W316 T317 R323 D330 C337 H338 S339 D344 T351 H367 W368 I369 E372 G373 T378 GLN ASN PRO L382 N386 L397 E400 Q407 A420 M427

I431 W434 K439 R440 P441 R445 HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.09Å 94.03Å 155.20Å 101.47° 96.74° 79.86°	Depositor
Resolution (Å)	19.86 – 2.80 19.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.86-2.80) 97.6 (19.86-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.8_1066	Depositor
R, R_{free}	0.173 , 0.231 0.175 , 0.233	Depositor DCC
R_{free} test set	5611 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27172	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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 (i)

5.1 Standard geometry (i)

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

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	0.46	0/3479	0.67	2/4736 (0.0%)
1	B	0.47	1/3479 (0.0%)	0.63	1/4736 (0.0%)
1	C	0.45	1/3479 (0.0%)	0.63	0/4736
1	D	0.43	0/3353	0.61	0/4565
1	E	0.47	0/3300	0.63	0/4493
1	F	0.43	0/3473	0.61	0/4727
1	G	0.43	0/3291	0.60	0/4480
1	H	0.40	0/3360	0.61	0/4567
All	All	0.44	2/27214 (0.0%)	0.63	3/37040 (0.0%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	CYS	CB-SG	-5.34	1.73	1.81
1	B	165	GLU	CD-OE2	-5.24	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	165	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	A	189	ARG	NE-CZ-NH2	-5.29	117.66	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	189	ARG	Sidechain

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	3396	0	3331	57	0
1	B	3396	0	3331	39	0
1	C	3396	0	3331	53	0
1	D	3275	0	3223	39	0
1	E	3224	0	3176	32	0
1	F	3390	0	3327	42	0
1	G	3215	0	3166	32	0
1	H	3283	0	3222	49	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	1	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
2	G	13	0	5	1	0
2	H	13	0	5	0	0
3	E	6	0	8	3	0
3	G	6	0	8	0	0
4	A	71	0	0	5	0
4	B	74	0	0	3	0
4	C	70	0	0	2	0
4	D	68	0	0	2	0
4	E	68	0	0	2	0
4	F	59	0	0	2	0
4	G	41	0	0	1	0
4	H	30	0	0	4	0
All	All	27172	0	26163	318	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 (318) 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:97:THR:HG21	1:A:108:ARG:HH22	1.43	0.82
1:A:43:THR:HG22	1:A:49:THR:HG22	1.61	0.82
1:H:439:LYS:O	1:H:445:ARG:NH2	2.16	0.79
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.48	0.79
1:D:107:LEU:O	1:D:110:ASN:ND2	2.20	0.73
1:H:274:MET:HG3	1:H:290:ILE:HD13	1.71	0.73
1:H:36:THR:HG23	1:H:56:GLY:HA3	1.71	0.72
1:H:439:LYS:HE2	4:H:611:HOH:O	1.88	0.72
1:G:274:MET:HG3	1:G:290:ILE:HD13	1.72	0.71
1:A:248:CYS:HA	1:A:251:LEU:HD12	1.72	0.70
1:A:261:PRO:HD2	1:A:274:MET:HE1	1.72	0.70
1:G:323:ARG:NH2	1:H:330:ASP:OD2	2.25	0.69
1:B:330:ASP:OD2	1:E:323:ARG:NH2	2.26	0.69
1:C:65:VAL:HA	1:C:68:ILE:HD12	1.74	0.69
1:H:386:ASN:ND2	4:H:626:HOH:O	2.26	0.67
1:E:274:MET:HG3	1:E:290:ILE:HD13	1.77	0.66
1:H:55:PRO:HD2	1:H:110:ASN:HB3	1.76	0.66
1:A:249:LYS:HA	4:A:610:HOH:O	1.94	0.66
1:B:167:THR:HG23	1:B:174:TYR:HB3	1.77	0.66
1:A:344:ASP:OD2	1:A:378:THR:OG1	2.11	0.66
1:H:431:ILE:HG13	1:H:431:ILE:O	1.94	0.65
1:D:54:ALA:HB2	1:D:114:ALA:HB2	1.78	0.65
1:A:274:MET:HG3	1:A:290:ILE:HD13	1.79	0.65
1:H:252:ASN:ND2	4:H:627:HOH:O	2.24	0.65
1:B:274:MET:HG3	1:B:290:ILE:HD13	1.79	0.65
1:C:123:LEU:HD23	1:C:134:LEU:HD13	1.79	0.64
1:D:87:HIS:O	1:D:87:HIS:ND1	2.31	0.64
1:E:6:SER:N	4:E:639:HOH:O	2.31	0.64
1:H:264:ALA:O	1:H:439:LYS:NZ	2.31	0.63
1:A:137:PRO:HB3	1:F:84:GLN:HG3	1.79	0.63
1:F:54:ALA:HB2	1:F:114:ALA:HB2	1.80	0.63
1:B:230:ARG:H	1:B:230:ARG:HD2	1.63	0.63
1:G:330:ASP:OD2	1:H:323:ARG:NH2	2.32	0.63
1:H:9:ILE:HG21	1:H:71:VAL:HG12	1.80	0.62
1:G:54:ALA:HB2	1:G:114:ALA:HB2	1.80	0.61
1:C:32:ASN:OD1	4:C:613:HOH:O	2.15	0.61
1:E:171:HIS:HE1	3:E:502:GOL:H31	1.63	0.61
1:C:304:ASN:OD1	1:H:279:ARG:NH2	2.34	0.60
1:C:81:LYS:O	1:C:85:GLN:HG3	2.01	0.60
1:G:17:VAL:HG13	1:G:409:ALA:HB1	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:HD12	1:D:345:ILE:HD12	1.83	0.59
1:F:123:LEU:HD23	1:F:134:LEU:HD13	1.84	0.59
1:C:54:ALA:HB2	1:C:114:ALA:HB2	1.84	0.59
1:B:202:ASP:OD1	1:B:230:ARG:HD3	2.01	0.59
1:B:338:HIS:HB3	4:B:617:HOH:O	2.03	0.59
1:H:83:VAL:HG11	1:H:116:GLU:HG3	1.84	0.59
1:F:278:ARG:NH2	1:F:307:ASP:OD1	2.31	0.59
1:D:167:THR:O	1:D:175:GLN:NE2	2.36	0.58
1:B:248:CYS:HA	1:B:251:LEU:HD12	1.85	0.58
1:A:130:PRO:HG3	1:A:393:ASP:HA	1.84	0.58
1:B:55:PRO:HD2	1:B:110:ASN:HB3	1.86	0.58
1:H:54:ALA:HB2	1:H:114:ALA:HB2	1.86	0.58
1:A:137:PRO:CB	1:F:84:GLN:HG3	2.33	0.57
1:B:262:CYS:HB3	4:B:601:HOH:O	2.04	0.57
1:C:98:PHE:HB2	1:C:107:LEU:HD21	1.86	0.57
1:D:274:MET:HG3	1:D:290:ILE:HD13	1.85	0.57
1:C:279:ARG:NH2	1:H:304:ASN:HD21	2.03	0.57
1:A:62:GLN:HA	1:A:65:VAL:HG22	1.85	0.57
1:A:304:ASN:ND2	1:E:304:ASN:OD1	2.38	0.57
1:H:36:THR:CG2	1:H:56:GLY:HA3	2.35	0.56
1:D:235:PRO:HG2	1:D:261:PRO:HA	1.87	0.56
1:A:87:HIS:O	1:A:87:HIS:ND1	2.37	0.56
1:E:344:ASP:OD2	1:E:378:THR:OG1	2.14	0.56
1:G:60:ILE:HG13	4:G:608:HOH:O	2.06	0.56
1:H:368:TRP:NE1	1:H:372:GLU:OE1	2.39	0.56
1:A:54:ALA:HB2	1:A:114:ALA:HB2	1.86	0.56
1:C:235:PRO:HG2	1:C:261:PRO:HA	1.87	0.56
1:B:167:THR:HG21	1:B:177:ARG:NH2	2.21	0.55
1:E:171:HIS:CE1	3:E:502:GOL:H31	2.41	0.55
1:E:147:LEU:HD11	1:E:365:ASP:HA	1.87	0.54
1:A:97:THR:HG21	4:A:649:HOH:O	2.06	0.54
1:C:175:GLN:HG2	1:E:403:TRP:CE2	2.42	0.54
1:C:330:ASP:OD2	1:D:323:ARG:NH2	2.40	0.54
1:E:287:THR:OG1	1:E:290:ILE:HG12	2.06	0.54
1:E:9:ILE:HG21	1:E:71:VAL:HG12	1.89	0.54
1:F:271:ARG:HA	1:F:290:ILE:HD12	1.89	0.54
1:F:382:LEU:HD21	1:F:392:PRO:HG3	1.89	0.54
1:H:313:PRO:HD3	1:H:337:CYS:SG	2.48	0.54
1:A:94:ASP:OD1	1:A:108:ARG:HG3	2.08	0.54
1:C:84:GLN:HG3	1:C:88:LYS:HZ2	1.73	0.53
1:H:278:ARG:NH1	1:H:304:ASN:OD1	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:GLN:HB2	1:F:203:PHE:HZ	1.73	0.53
1:F:437:ASP:HB3	1:F:440:ARG:HB3	1.89	0.53
1:C:189:ARG:HD2	1:E:407:GLN:HG2	1.90	0.53
1:A:156:ARG:HG2	4:A:633:HOH:O	2.07	0.53
1:B:30:ALA:HB3	1:B:426:PRO:HB2	1.91	0.53
1:B:87:HIS:HD2	1:B:109:VAL:HG23	1.73	0.53
1:D:144:ILE:HD13	1:D:351:THR:HA	1.90	0.53
1:F:17:VAL:HB	1:F:409:ALA:HB1	1.91	0.53
1:B:246:SER:O	1:B:249:LYS:HB2	2.10	0.52
1:G:288:ASN:O	1:G:292:THR:HG22	2.08	0.52
1:A:144:ILE:HD13	1:A:351:THR:HA	1.90	0.52
1:F:84:GLN:NE2	1:F:88:LYS:HE2	2.23	0.52
1:B:87:HIS:CD2	1:B:109:VAL:HG23	2.44	0.52
1:C:84:GLN:HE21	1:C:88:LYS:HZ1	1.58	0.52
1:D:27:ILE:HD12	1:D:238:ALA:HB2	1.91	0.52
1:B:110:ASN:HA	1:B:314:HIS:O	2.10	0.51
1:H:230:ARG:HD3	1:H:230:ARG:N	2.25	0.51
1:D:107:LEU:HG	1:D:109:VAL:HG12	1.92	0.51
1:F:335:TRP:CH2	1:F:337:CYS:HB2	2.46	0.51
1:D:431:ILE:HD11	1:D:443:PHE:CD1	2.46	0.51
1:D:248:CYS:HA	1:D:251:LEU:HD12	1.92	0.51
1:H:248:CYS:HA	1:H:251:LEU:HD12	1.93	0.51
1:C:144:ILE:HD13	1:C:351:THR:HA	1.93	0.51
1:G:437:ASP:HB3	1:G:440:ARG:HB3	1.93	0.51
1:A:311:ALA:HB3	1:A:335:TRP:HE1	1.76	0.50
1:F:79:LEU:HA	1:F:82:VAL:HG12	1.93	0.50
1:C:294:TRP:HB3	1:D:330:ASP:HB3	1.92	0.50
1:D:11:ASP:HB3	1:D:43:THR:OG1	2.12	0.50
1:F:144:ILE:HD13	1:F:351:THR:HA	1.93	0.50
1:F:278:ARG:HG3	1:F:285:VAL:HG13	1.94	0.50
1:C:17:VAL:HG23	1:C:37:ARG:HB2	1.92	0.50
1:C:263:GLY:H	1:C:439:LYS:NZ	2.09	0.50
1:D:108:ARG:HG3	1:D:108:ARG:HH11	1.76	0.50
1:E:84:GLN:O	1:E:87:HIS:HB3	2.11	0.50
1:A:171:HIS:CD2	1:A:197:ARG:HD3	2.47	0.50
1:D:431:ILE:HD11	1:D:443:PHE:CE1	2.46	0.50
1:H:169:GLY:HA3	1:H:174:TYR:HD2	1.76	0.50
1:H:427:MET:HG3	1:H:434:TRP:CD2	2.47	0.50
1:H:110:ASN:HA	1:H:314:HIS:O	2.12	0.50
1:F:93:ALA:O	1:F:97:THR:HG23	2.11	0.50
1:H:274:MET:HE2	1:H:285:VAL:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LEU:HD12	1:D:108:ARG:H	1.77	0.50
1:E:87:HIS:O	1:E:87:HIS:ND1	2.45	0.50
1:G:287:THR:OG1	1:G:290:ILE:HG12	2.11	0.49
1:H:192:GLU:OE2	1:H:225:ARG:NE	2.33	0.49
1:E:107:LEU:HD13	1:E:315:PHE:HE1	1.77	0.49
1:E:171:HIS:ND1	3:E:502:GOL:H11	2.26	0.49
1:D:110:ASN:HA	1:D:314:HIS:O	2.12	0.49
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.76	0.49
1:A:330:ASP:OD2	1:F:323:ARG:NH2	2.46	0.49
1:B:230:ARG:HD2	1:B:230:ARG:N	2.26	0.49
1:C:130:PRO:HG3	1:C:393:ASP:HA	1.94	0.49
1:A:294:TRP:HB3	1:F:330:ASP:HB3	1.94	0.49
1:C:84:GLN:HE21	1:C:88:LYS:NZ	2.10	0.49
1:F:235:PRO:HG2	1:F:261:PRO:HA	1.95	0.49
1:B:144:ILE:HD13	1:B:351:THR:HA	1.94	0.49
1:A:65:VAL:HA	1:A:68:ILE:HD12	1.94	0.49
1:A:316:TRP:O	1:A:317:THR:OG1	2.25	0.48
1:C:274:MET:HG3	1:C:290:ILE:HD13	1.95	0.48
1:H:173:TRP:CZ2	1:H:369:ILE:HG23	2.48	0.48
1:A:84:GLN:HG3	1:F:137:PRO:CB	2.44	0.48
1:D:107:LEU:HD12	1:D:108:ARG:N	2.28	0.48
1:B:39:ILE:HD12	1:B:345:ILE:HD12	1.95	0.48
1:C:94:ASP:OD1	1:C:108:ARG:HG3	2.13	0.48
1:C:240:LEU:HD23	1:C:439:LYS:HD2	1.95	0.48
1:F:388:LYS:HE2	4:F:656:HOH:O	2.13	0.48
1:F:241:LEU:N	1:F:265:GLU:OE2	2.37	0.48
1:G:130:PRO:HG3	1:G:393:ASP:HA	1.96	0.48
1:A:38:ASN:OD1	1:A:56:GLY:HA2	2.14	0.48
1:D:131:VAL:HG23	1:D:396:GLY:C	2.34	0.48
1:D:55:PRO:HD2	1:D:110:ASN:HB3	1.96	0.48
1:A:96:ASP:O	1:A:100:LYS:HG3	2.13	0.47
1:F:343:PHE:CD1	1:F:377:LEU:HG	2.49	0.47
1:A:269:SER:HB3	1:B:269:SER:HB3	1.95	0.47
1:B:27:ILE:HD12	1:B:238:ALA:HB2	1.97	0.47
1:C:437:ASP:HB3	1:C:440:ARG:HB3	1.96	0.47
1:F:55:PRO:HD2	1:F:110:ASN:HB3	1.95	0.47
1:G:28:GLY:HA2	1:G:436:PHE:CD1	2.50	0.47
1:A:9:ILE:HD11	1:A:71:VAL:O	2.13	0.47
1:A:261:PRO:HD2	1:A:274:MET:CE	2.44	0.47
1:G:11:ASP:HB3	1:G:43:THR:HG22	1.96	0.47
1:G:159:THR:HG22	1:G:429:TYR:CB	2.45	0.47

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH2	4:A:649:HOH:O	2.47	0.47
1:B:86:VAL:HG12	1:B:112:VAL:HG22	1.96	0.47
1:C:175:GLN:HG2	1:E:403:TRP:CD2	2.49	0.47
1:H:316:TRP:O	1:H:317:THR:OG1	2.24	0.47
1:C:61:TYR:O	1:C:65:VAL:HG23	2.14	0.47
1:D:312:ASP:HB2	1:D:338:HIS:HB3	1.97	0.47
1:G:340:ASN:O	1:G:342:HIS:HD2	1.97	0.47
2:C:501:CIT:H42	2:C:501:CIT:O1	2.13	0.47
1:F:249:LYS:HA	4:F:606:HOH:O	2.14	0.47
1:F:261:PRO:HD2	1:F:274:MET:HE1	1.96	0.47
1:A:96:ASP:OD1	1:B:266:GLN:NE2	2.47	0.47
1:C:39:ILE:HD12	1:C:345:ILE:HD12	1.97	0.47
1:C:196:ASP:OD1	1:E:414:LYS:NZ	2.33	0.47
1:D:292:THR:HA	4:D:601:HOH:O	2.15	0.46
1:G:140:GLN:OE1	1:H:84:GLN:NE2	2.48	0.46
1:H:235:PRO:HG2	1:H:261:PRO:HA	1.97	0.46
1:A:84:GLN:HG3	1:F:137:PRO:HB2	1.96	0.46
1:B:130:PRO:HG3	1:B:393:ASP:HA	1.96	0.46
1:G:173:TRP:CZ2	1:G:369:ILE:HG13	2.51	0.46
1:H:27:ILE:HD12	1:H:238:ALA:HB2	1.97	0.46
1:C:98:PHE:HA	1:C:102:ALA:HB3	1.96	0.46
1:F:62:GLN:HA	1:F:65:VAL:HG23	1.97	0.46
1:A:127:LEU:HD22	1:F:77:ALA:HB2	1.97	0.46
1:B:54:ALA:HB2	1:B:114:ALA:HB2	1.98	0.46
1:C:241:LEU:N	1:C:265:GLU:OE2	2.47	0.46
1:D:335:TRP:CH2	1:D:337:CYS:HB2	2.51	0.46
1:A:271:ARG:HA	1:A:290:ILE:HD12	1.97	0.46
1:D:105:PHE:CE1	1:D:421:ARG:HD3	2.51	0.46
1:E:249:LYS:NZ	4:E:666:HOH:O	2.49	0.46
1:G:158:LYS:HE3	1:G:158:LYS:HB3	1.42	0.46
1:C:6:SER:N	1:C:7:PRO:CD	2.78	0.46
1:H:278:ARG:HG3	1:H:285:VAL:HG13	1.98	0.46
1:A:9:ILE:HD12	1:A:71:VAL:HG12	1.97	0.45
1:B:78:ARG:NH1	1:E:133:GLU:OE2	2.48	0.45
1:B:287:THR:HG22	1:B:290:ILE:HD11	1.98	0.45
1:C:343:PHE:CD1	1:C:377:LEU:HG	2.51	0.45
1:H:85:GLN:HG2	1:H:88:LYS:HD3	1.98	0.45
1:E:259:GLU:HA	1:E:286:ALA:O	2.16	0.45
1:E:288:ASN:O	1:E:292:THR:HG22	2.17	0.45
1:C:269:SER:HB3	1:G:269:SER:HB3	1.98	0.45
1:D:329:ASP:OD1	1:D:359:GLY:HA3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:PHE:HA	1:H:102:ALA:HB3	1.97	0.45
1:H:241:LEU:N	1:H:265:GLU:OE2	2.41	0.45
1:A:42:LEU:HD11	1:A:115:LEU:HD12	1.99	0.45
1:B:96:ASP:O	4:B:646:HOH:O	2.21	0.45
1:C:263:GLY:H	1:C:439:LYS:HZ3	1.65	0.45
1:C:382:LEU:HG	4:C:616:HOH:O	2.16	0.45
1:E:248:CYS:HA	1:E:251:LEU:HD12	1.97	0.45
1:B:65:VAL:HA	1:B:68:ILE:HD12	1.99	0.45
1:C:179:GLN:HE21	1:C:179:GLN:HB3	1.44	0.45
1:F:355:ALA:HB2	1:F:391:VAL:HG21	1.98	0.45
1:H:96:ASP:O	4:H:625:HOH:O	2.21	0.45
1:H:344:ASP:OD1	1:H:344:ASP:N	2.38	0.45
1:B:184:SER:OG	1:B:218:THR:HA	2.17	0.45
1:D:83:VAL:HG21	1:D:116:GLU:HG3	1.99	0.45
1:G:248:CYS:HA	1:G:251:LEU:HD12	1.99	0.45
1:B:98:PHE:HB2	1:B:107:LEU:HD21	1.99	0.44
1:D:198:TYR:HB2	1:D:200:PHE:CE2	2.52	0.44
1:A:315:PHE:HZ	1:A:340:ASN:HD22	1.64	0.44
1:A:434:TRP:O	4:A:661:HOH:O	2.21	0.44
1:D:235:PRO:HD2	1:D:259:GLU:O	2.17	0.44
1:A:234:ASP:HB2	1:A:259:GLU:HB3	1.99	0.44
1:C:248:CYS:HA	1:C:251:LEU:HD12	1.99	0.44
1:F:337:CYS:HB3	1:F:364:ILE:HG12	1.98	0.44
1:A:61:TYR:O	1:A:65:VAL:HG13	2.18	0.44
1:C:110:ASN:HA	1:C:314:HIS:O	2.17	0.44
1:C:257:TYR:CD2	1:C:308:ILE:HD13	2.53	0.44
1:E:10:THR:OG1	1:E:43:THR:HG22	2.17	0.44
1:A:153:ILE:HD11	1:A:370:TRP:CH2	2.52	0.44
1:A:195:GLN:HB2	1:A:203:PHE:HZ	1.82	0.44
1:B:310:LEU:HD22	1:B:336:GLY:HA3	2.00	0.44
1:C:84:GLN:CG	1:C:88:LYS:HZ2	2.30	0.44
1:C:176:LEU:HD23	1:C:176:LEU:HA	1.86	0.44
1:C:312:ASP:HB2	1:C:338:HIS:HB3	2.00	0.44
1:E:173:TRP:CZ2	1:E:369:ILE:HG13	2.53	0.44
1:B:279:ARG:NH2	1:F:304:ASN:OD1	2.51	0.44
1:H:65:VAL:HA	1:H:68:ILE:HD12	2.00	0.44
1:D:81:LYS:HE3	4:D:620:HOH:O	2.17	0.43
1:G:147:LEU:HD11	1:G:365:ASP:HA	1.99	0.43
1:D:309:PRO:HG2	1:D:328:CYS:SG	2.58	0.43
1:H:131:VAL:HG21	1:H:397:LEU:HD23	1.99	0.43
1:A:79:LEU:HA	1:A:82:VAL:HG12	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:CYS:HB3	1:A:364:ILE:HG23	2.01	0.43
1:E:140:GLN:HG3	1:E:358:PRO:HA	2.01	0.43
1:G:200:PHE:CZ	1:G:369:ILE:HG21	2.52	0.43
1:H:198:TYR:CE2	1:H:369:ILE:HD12	2.53	0.43
1:E:64:LEU:HG	1:E:111:ALA:HB1	2.01	0.43
1:A:29:GLY:HA2	1:A:427:MET:HG2	2.00	0.43
1:F:362:THR:OG1	1:F:363:ALA:N	2.51	0.43
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.23	0.43
1:D:313:PRO:HD3	1:D:337:CYS:SG	2.59	0.43
1:H:339:SER:HG	1:H:367:HIS:HD1	1.65	0.43
1:G:17:VAL:HG11	1:G:377:LEU:HD11	2.00	0.43
1:F:76:VAL:HG12	1:F:123:LEU:HD13	2.00	0.43
1:G:10:THR:OG1	1:G:43:THR:HG23	2.19	0.43
1:A:81:LYS:O	1:A:85:GLN:HG3	2.19	0.42
1:A:67:ALA:O	1:A:71:VAL:HG23	2.19	0.42
1:C:132:CYS:O	1:C:138:GLY:HA2	2.19	0.42
1:C:410:HIS:O	1:C:414:LYS:HG3	2.19	0.42
1:F:8:VAL:HB	1:F:45:ASN:ND2	2.35	0.42
1:F:65:VAL:HA	1:F:68:ILE:HD12	2.01	0.42
1:F:28:GLY:HA2	1:F:436:PHE:CD1	2.55	0.42
1:F:312:ASP:HB2	1:F:338:HIS:HB3	2.01	0.42
1:C:333:LEU:HD23	1:C:333:LEU:HA	1.84	0.42
1:F:224:LYS:HE3	1:F:224:LYS:HB3	1.76	0.42
1:D:70:MET:SD	1:D:86:VAL:HG22	2.60	0.42
1:H:144:ILE:HD13	1:H:351:THR:HA	2.02	0.42
1:E:110:ASN:HA	1:E:314:HIS:O	2.20	0.42
1:G:19:GLY:O	1:G:34:TYR:HA	2.19	0.42
1:H:23:MET:SD	1:H:154:GLY:HA3	2.60	0.42
1:B:230:ARG:HB3	1:B:256:THR:OG1	2.19	0.42
1:F:94:ASP:OD1	1:F:108:ARG:HG3	2.19	0.42
1:H:312:ASP:HB2	1:H:338:HIS:HB3	2.02	0.41
1:G:177:ARG:NH2	1:G:374:ASP:OD2	2.49	0.41
1:G:235:PRO:HG2	1:G:261:PRO:HA	2.03	0.41
1:H:84:GLN:HG3	1:H:85:GLN:N	2.34	0.41
1:H:283:LEU:HD23	1:H:283:LEU:HA	1.86	0.41
1:C:107:LEU:O	1:C:110:ASN:ND2	2.53	0.41
1:C:343:PHE:CE1	1:C:375:CYS:HB3	2.55	0.41
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.85	0.41
1:A:315:PHE:HZ	1:A:340:ASN:ND2	2.19	0.41
1:E:144:ILE:HD13	1:E:351:THR:HA	2.02	0.41
1:B:437:ASP:HB3	1:B:440:ARG:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.93	0.41
1:D:316:TRP:O	1:D:317:THR:OG1	2.27	0.41
1:E:55:PRO:HD2	1:E:110:ASN:HB3	2.02	0.41
1:E:189:ARG:HD3	1:E:192:GLU:OE1	2.21	0.41
1:B:307:ASP:C	1:B:308:ILE:HG13	2.40	0.41
1:G:159:THR:HG22	1:G:429:TYR:HB2	2.01	0.41
1:G:344:ASP:OD1	1:G:344:ASP:N	2.51	0.41
1:G:427:MET:HG3	1:G:434:TRP:CD2	2.56	0.41
1:B:330:ASP:HB3	1:E:294:TRP:HB3	2.03	0.41
1:C:195:GLN:HB2	1:C:203:PHE:HZ	1.86	0.41
1:G:197:ARG:HD2	1:G:197:ARG:O	2.21	0.41
1:B:235:PRO:HG2	1:B:261:PRO:HA	2.03	0.41
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.81	0.41
1:D:11:ASP:OD2	1:D:13:LYS:NZ	2.54	0.41
1:F:131:VAL:HG21	1:F:397:LEU:HD23	2.02	0.41
1:G:144:ILE:HD13	1:G:351:THR:HA	2.02	0.41
1:H:208:GLY:O	1:H:441:PRO:HA	2.21	0.41
1:H:251:LEU:HD23	1:H:251:LEU:HA	1.82	0.41
1:A:94:ASP:OD1	1:A:108:ARG:NH1	2.47	0.41
1:C:79:LEU:O	1:C:83:VAL:HG23	2.20	0.41
1:D:344:ASP:OD1	1:D:344:ASP:N	2.44	0.41
1:A:260:ASP:HA	1:A:274:MET:HE2	2.03	0.40
1:B:431:ILE:HB	1:B:434:TRP:HB2	2.03	0.40
1:F:107:LEU:O	1:F:110:ASN:ND2	2.53	0.40
1:A:9:ILE:CD1	1:A:71:VAL:HG12	2.51	0.40
1:C:335:TRP:CH2	1:C:337:CYS:HB2	2.56	0.40
1:C:337:CYS:HB3	1:C:364:ILE:HG23	2.04	0.40
1:G:161:LEU:N	1:G:161:LEU:HD12	2.36	0.40
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.89	0.40
1:D:16:PRO:HB2	1:D:413:TYR:CD2	2.56	0.40
2:G:501:CIT:H42	2:G:501:CIT:O2	2.22	0.40
1:C:330:ASP:HB3	1:D:294:TRP:HB3	2.04	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	438/466 (94%)	429 (98%)	8 (2%)	1 (0%)	47	78
1	B	438/466 (94%)	427 (98%)	10 (2%)	1 (0%)	47	78
1	C	438/466 (94%)	429 (98%)	9 (2%)	0	100	100
1	D	420/466 (90%)	409 (97%)	10 (2%)	1 (0%)	47	78
1	E	411/466 (88%)	405 (98%)	6 (2%)	0	100	100
1	F	437/466 (94%)	431 (99%)	5 (1%)	1 (0%)	47	78
1	G	410/466 (88%)	401 (98%)	8 (2%)	1 (0%)	47	78
1	H	420/466 (90%)	415 (99%)	4 (1%)	1 (0%)	47	78
All	All	3412/3728 (92%)	3346 (98%)	60 (2%)	6 (0%)	47	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	156	ARG
1	A	156	ARG
1	B	156	ARG
1	D	156	ARG
1	G	156	ARG
1	F	156	ARG

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	350/372 (94%)	332 (95%)	18 (5%)	24	55
1	B	350/372 (94%)	339 (97%)	11 (3%)	40	74
1	C	350/372 (94%)	338 (97%)	12 (3%)	37	71
1	D	340/372 (91%)	323 (95%)	17 (5%)	24	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	336/372 (90%)	319 (95%)	17 (5%)	24	55
1	F	349/372 (94%)	331 (95%)	18 (5%)	23	55
1	G	334/372 (90%)	319 (96%)	15 (4%)	27	60
1	H	336/372 (90%)	322 (96%)	14 (4%)	30	63
All	All	2745/2976 (92%)	2623 (96%)	122 (4%)	28	61

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	88	LYS
1	A	104	THR
1	A	108	ARG
1	A	149	TYR
1	A	170	ASN
1	A	184	SER
1	A	189	ARG
1	A	230	ARG
1	A	262	CYS
1	A	265	GLU
1	A	339	SER
1	A	360	ASN
1	A	380	ASN
1	A	382	LEU
1	A	427	MET
1	A	438	ARG
1	A	445	ARG
1	B	17	VAL
1	B	149	TYR
1	B	165	GLU
1	B	170	ASN
1	B	184	SER
1	B	249	LYS
1	B	262	CYS
1	B	339	SER
1	B	374	ASP
1	B	427	MET
1	B	445	ARG
1	C	6	SER
1	C	62	GLN
1	C	87	HIS

Continued on next page...

Full wwPDB X-ray Structure Validation Report 4IL0

Continued from previous page...

Mol	Chain	Res	Type
1	C	108	ARG
1	C	149	TYR
1	C	179	GLN
1	C	184	SER
1	C	194	SER
1	C	230	ARG
1	C	262	CYS
1	C	427	MET
1	C	445	ARG
1	D	43	THR
1	D	62	GLN
1	D	65	VAL
1	D	70	MET
1	D	84	GLN
1	D	87	HIS
1	D	108	ARG
1	D	149	TYR
1	D	185	GLU
1	D	194	SER
1	D	230	ARG
1	D	249	LYS
1	D	262	CYS
1	D	279	ARG
1	D	339	SER
1	D	438	ARG
1	D	445	ARG
1	E	6	SER
1	E	62	GLN
1	E	81	LYS
1	E	84	GLN
1	E	87	HIS
1	E	107	LEU
1	E	108	ARG
1	E	149	TYR
1	E	184	SER
1	E	194	SER
1	E	230	ARG
1	E	249	LYS
1	E	262	CYS
1	E	279	ARG
1	E	407	GLN
1	E	427	MET

Continued from previous page...

Mol	Chain	Res	Type
1	E	445	ARG
1	F	43	THR
1	F	62	GLN
1	F	65	VAL
1	F	85	GLN
1	F	87	HIS
1	F	108	ARG
1	F	149	TYR
1	F	158	LYS
1	F	180	LYS
1	F	189	ARG
1	F	195	GLN
1	F	230	ARG
1	F	249	LYS
1	F	262	CYS
1	F	285	VAL
1	F	427	MET
1	F	439	LYS
1	F	445	ARG
1	G	43	THR
1	G	62	GLN
1	G	87	HIS
1	G	149	TYR
1	G	158	LYS
1	G	180	LYS
1	G	195	GLN
1	G	230	ARG
1	G	249	LYS
1	G	339	SER
1	G	369	ILE
1	G	407	GLN
1	G	427	MET
1	G	438	ARG
1	G	445	ARG
1	H	17	VAL
1	H	36	THR
1	H	39	ILE
1	H	84	GLN
1	H	87	HIS
1	H	149	TYR
1	H	156	ARG
1	H	230	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	233	VAL
1	H	339	SER
1	H	369	ILE
1	H	427	MET
1	H	431	ILE
1	H	445	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	340	ASN
1	B	87	HIS
1	C	84	GLN
1	C	266	GLN
1	D	360	ASN
1	E	38	ASN
1	F	166	ASN
1	F	179	GLN
1	G	140	GLN
1	H	84	GLN

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 ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CIT	G	501	-	12,12,12	1.05	0	17,17,17	1.99	5 (29%)
2	CIT	A	501	-	12,12,12	1.20	1 (8%)	17,17,17	2.08	4 (23%)
2	CIT	H	501	-	12,12,12	0.99	0	17,17,17	1.60	4 (23%)
2	CIT	D	501	-	12,12,12	0.99	0	17,17,17	1.71	5 (29%)
2	CIT	C	501	-	12,12,12	1.10	0	17,17,17	2.26	10 (58%)
3	GOL	G	502	-	5,5,5	0.32	0	5,5,5	0.63	0
2	CIT	F	501	-	12,12,12	1.10	0	17,17,17	1.84	7 (41%)
3	GOL	E	502	-	5,5,5	0.39	0	5,5,5	0.32	0
2	CIT	B	501	-	12,12,12	1.16	1 (8%)	17,17,17	1.77	5 (29%)
2	CIT	E	501	-	12,12,12	1.11	0	17,17,17	1.70	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	G	501	-	-	2/16/16/16	-
2	CIT	A	501	-	-	8/16/16/16	-
2	CIT	H	501	-	-	3/16/16/16	-
2	CIT	D	501	-	-	2/16/16/16	-
2	CIT	C	501	-	-	12/16/16/16	-
3	GOL	G	502	-	-	4/4/4/4	-
2	CIT	F	501	-	-	2/16/16/16	-
3	GOL	E	502	-	-	4/4/4/4	-
2	CIT	B	501	-	-	5/16/16/16	-
2	CIT	E	501	-	-	5/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CIT	C3-C6	-2.21	1.51	1.53
2	B	501	CIT	C3-C6	-2.03	1.51	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	CIT	C4-C3-C2	4.41	120.65	109.16
2	E	501	CIT	O6-C6-C3	4.29	120.50	113.05
2	C	501	CIT	O6-C6-C3	4.15	120.25	113.05
2	A	501	CIT	O6-C6-C3	4.05	120.08	113.05
2	G	501	CIT	O6-C6-C3	3.92	119.86	113.05
2	F	501	CIT	O6-C6-C3	3.71	119.50	113.05
2	D	501	CIT	O6-C6-C3	3.70	119.48	113.05
2	H	501	CIT	O6-C6-C3	3.50	119.14	113.05
2	C	501	CIT	C4-C3-C2	3.47	118.22	109.16
2	C	501	CIT	C4-C3-C6	-3.33	102.95	110.11
2	B	501	CIT	O6-C6-C3	3.00	118.25	113.05
2	F	501	CIT	O2-C1-C2	2.89	123.63	114.35
2	G	501	CIT	C4-C3-C6	-2.87	103.94	110.11
2	B	501	CIT	O2-C1-C2	2.82	123.39	114.35
2	B	501	CIT	C4-C3-C6	-2.80	104.10	110.11
2	D	501	CIT	O2-C1-C2	2.70	123.01	114.35
2	G	501	CIT	C3-C4-C5	-2.67	107.35	113.81
2	A	501	CIT	O4-C5-C4	2.64	122.82	114.35
2	C	501	CIT	C3-C2-C1	2.62	120.15	113.81
2	G	501	CIT	O2-C1-C2	2.61	122.73	114.35
2	G	501	CIT	C4-C3-C2	2.60	115.94	109.16
2	C	501	CIT	O4-C5-C4	2.57	122.60	114.35
2	A	501	CIT	O7-C3-C4	-2.55	103.43	109.40
2	C	501	CIT	O2-C1-O1	-2.49	117.10	123.30
2	C	501	CIT	O5-C6-C3	-2.45	118.79	122.25
2	C	501	CIT	O4-C5-O3	-2.43	117.24	123.30
2	H	501	CIT	O4-C5-O3	-2.38	117.36	123.30
2	D	501	CIT	O4-C5-C4	2.36	121.93	114.35
2	C	501	CIT	C3-C4-C5	-2.34	108.14	113.81
2	D	501	CIT	O4-C5-O3	-2.30	117.56	123.30
2	E	501	CIT	O5-C6-C3	-2.23	119.10	122.25
2	H	501	CIT	O7-C3-C6	2.22	111.98	108.86
2	F	501	CIT	O2-C1-O1	-2.18	117.86	123.30
2	F	501	CIT	O4-C5-O3	-2.18	117.86	123.30
2	H	501	CIT	O4-C5-C4	2.18	121.34	114.35
2	E	501	CIT	O2-C1-O1	-2.15	117.93	123.30
2	E	501	CIT	O2-C1-C2	2.14	121.22	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	CIT	O4-C5-C4	2.13	121.19	114.35
2	F	501	CIT	O5-C6-C3	-2.13	119.24	122.25
2	D	501	CIT	O2-C1-O1	-2.08	118.12	123.30
2	F	501	CIT	C4-C3-C6	-2.05	105.69	110.11
2	F	501	CIT	C2-C3-C6	-2.05	105.71	110.11
2	C	501	CIT	O7-C3-C2	-2.03	104.65	109.40
2	B	501	CIT	O2-C1-O1	-2.02	118.27	123.30

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C1-C2-C3-O7
2	A	501	CIT	C1-C2-C3-C4
2	A	501	CIT	C2-C3-C4-C5
2	A	501	CIT	O7-C3-C4-C5
2	C	501	CIT	C1-C2-C3-O7
2	C	501	CIT	C1-C2-C3-C4
2	C	501	CIT	C1-C2-C3-C6
2	E	501	CIT	C1-C2-C3-C4
2	E	501	CIT	C1-C2-C3-C6
2	H	501	CIT	C1-C2-C3-C4
2	H	501	CIT	C1-C2-C3-C6
3	E	502	GOL	O1-C1-C2-C3
3	G	502	GOL	C1-C2-C3-O3
3	G	502	GOL	O2-C2-C3-O3
2	H	501	CIT	C1-C2-C3-O7
2	A	501	CIT	C1-C2-C3-C6
3	G	502	GOL	O1-C1-C2-C3
2	A	501	CIT	C4-C3-C6-O6
3	E	502	GOL	O1-C1-C2-O2
3	G	502	GOL	O1-C1-C2-O2
2	A	501	CIT	C6-C3-C4-C5
2	B	501	CIT	O7-C3-C4-C5
2	B	501	CIT	C6-C3-C4-C5
2	C	501	CIT	O7-C3-C4-C5
2	C	501	CIT	C2-C3-C4-C5
2	E	501	CIT	C1-C2-C3-O7
2	C	501	CIT	O7-C3-C6-O6
2	C	501	CIT	C2-C3-C6-O6
2	C	501	CIT	C4-C3-C6-O6
2	B	501	CIT	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	501	CIT	C6-C3-C4-C5
2	B	501	CIT	O2-C1-C2-C3
2	B	501	CIT	C2-C3-C4-C5
2	A	501	CIT	C4-C3-C6-O5
2	C	501	CIT	C2-C3-C6-O5
2	E	501	CIT	C2-C3-C6-O6
2	G	501	CIT	O2-C1-C2-C3
2	D	501	CIT	O2-C1-C2-C3
2	F	501	CIT	O2-C1-C2-C3
2	F	501	CIT	O1-C1-C2-C3
2	G	501	CIT	O1-C1-C2-C3
2	D	501	CIT	O1-C1-C2-C3
2	E	501	CIT	C4-C3-C6-O6
3	E	502	GOL	O2-C2-C3-O3
3	E	502	GOL	C1-C2-C3-O3
2	C	501	CIT	C3-C4-C5-O3
2	C	501	CIT	C3-C4-C5-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	CIT	1	0
2	C	501	CIT	1	0
3	E	502	GOL	3	0

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, 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	440/466 (94%)	-0.67	5 (1%)	80	75	8, 21, 58, 98	0
1	B	440/466 (94%)	-0.75	0	100	100	10, 22, 45, 70	0
1	C	440/466 (94%)	-0.77	1 (0%)	95	94	10, 20, 42, 82	0
1	D	424/466 (90%)	-0.75	0	100	100	11, 23, 40, 73	0
1	E	417/466 (89%)	-0.77	0	100	100	9, 21, 37, 58	0
1	F	439/466 (94%)	-0.63	2 (0%)	91	88	9, 28, 53, 66	0
1	G	416/466 (89%)	-0.68	2 (0%)	91	88	12, 28, 45, 66	0
1	H	426/466 (91%)	-0.43	6 (1%)	75	70	13, 39, 61, 93	0
All	All	3442/3728 (92%)	-0.68	16 (0%)	91	88	8, 24, 53, 98	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	ASN	3.4
1	F	47	GLY	3.1
1	A	47	GLY	3.0
1	H	373	GLY	2.9
1	G	420	ALA	2.8
1	H	172	GLU	2.6
1	H	170	ASN	2.6
1	A	88	LYS	2.6
1	C	101	GLY	2.6
1	H	407	GLN	2.5
1	H	420	ALA	2.5
1	A	92	ALA	2.4
1	A	97	THR	2.2
1	H	400	GLU	2.1
1	F	101	GLY	2.1
1	G	168	PRO	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)

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, 95th 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
3	GOL	G	502	6/6	0.83	0.16	27,33,40,41	0
3	GOL	E	502	6/6	0.94	0.14	6,21,33,35	0
2	CIT	D	501	13/13	0.95	0.17	17,33,48,48	0
2	CIT	E	501	13/13	0.97	0.21	8,20,36,48	0
2	CIT	F	501	13/13	0.97	0.12	22,31,43,45	0
2	CIT	G	501	13/13	0.97	0.15	23,40,46,49	0
2	CIT	H	501	13/13	0.97	0.13	30,39,49,59	0
2	CIT	C	501	13/13	0.97	0.10	11,22,31,45	0
2	CIT	A	501	13/13	0.97	0.14	27,31,43,57	0
2	CIT	B	501	13/13	0.98	0.12	16,24,30,33	0

6.5 Other polymers (i)

There are no such residues in this entry.