Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:32 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

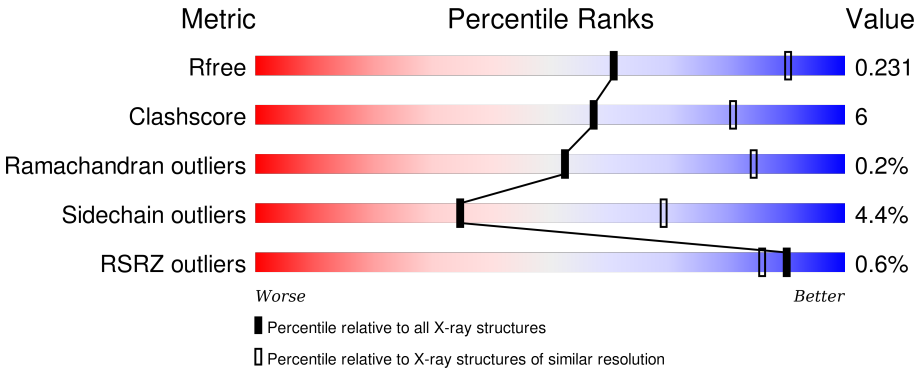
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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%

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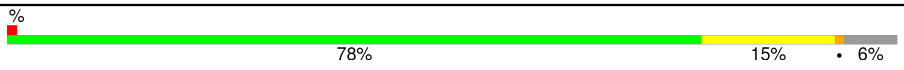
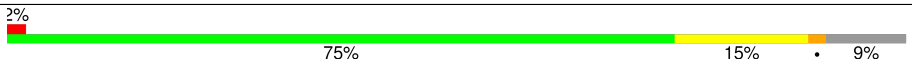
Mol	Chain	Length	Quality of chain
1	F	466	
1	G	466	
1	H	466	

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	E	501	-	-	-	X

2 Entry composition

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

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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

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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

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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

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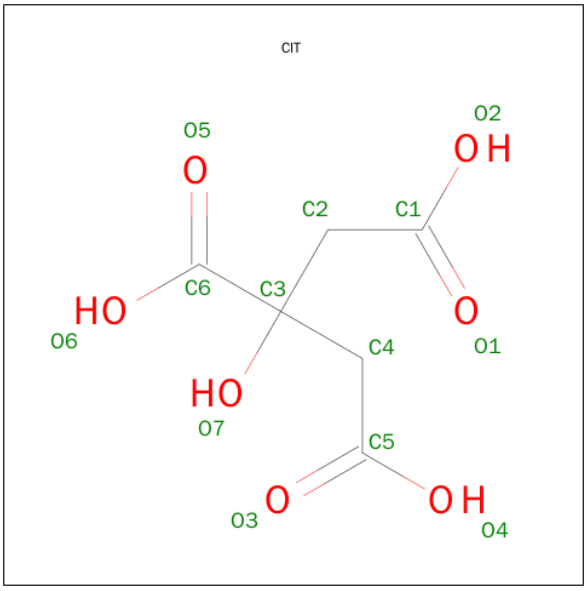
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP Q46915
H	-19	MET	-	EXPRESSION TAG	UNP Q46915
H	-18	GLY	-	EXPRESSION TAG	UNP Q46915
H	-17	SER	-	EXPRESSION TAG	UNP Q46915
H	-16	SER	-	EXPRESSION TAG	UNP Q46915
H	-15	HIS	-	EXPRESSION TAG	UNP Q46915
H	-14	HIS	-	EXPRESSION TAG	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	C	O	0	0
			13	6	7		

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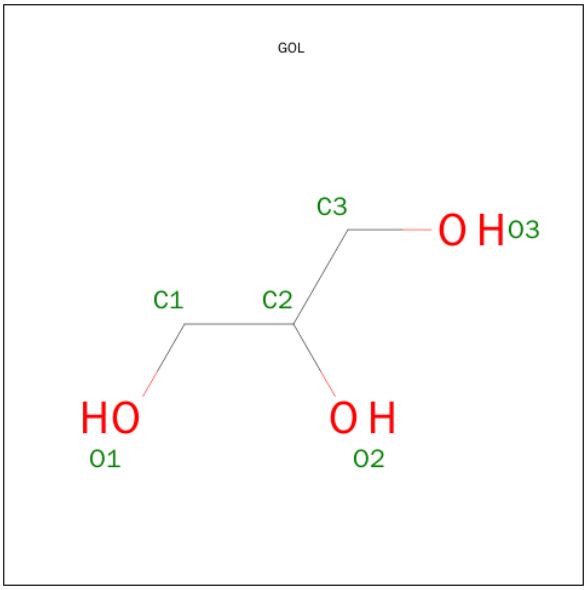
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

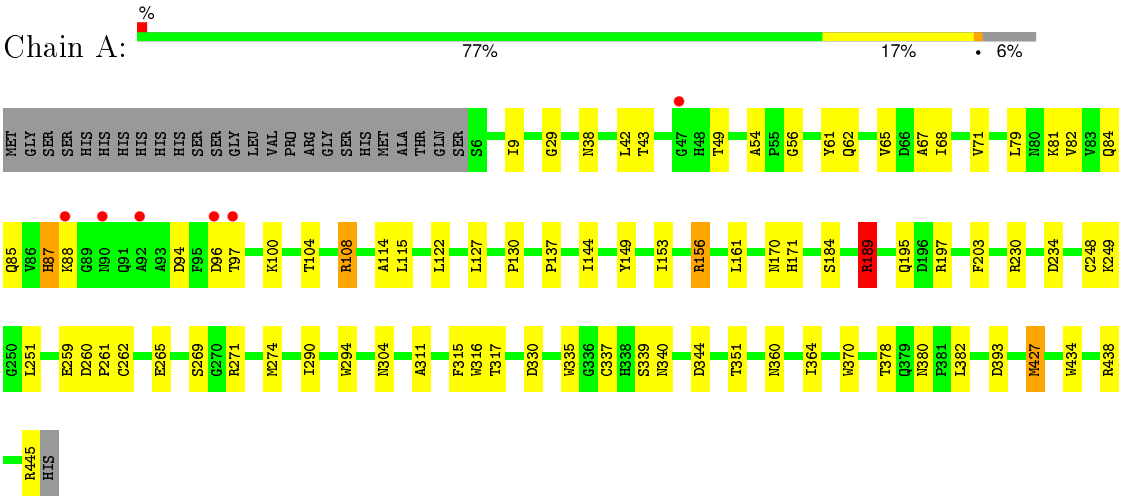
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	71	Total O 71 71	0	0
4	B	74	Total O 74 74	0	0
4	C	70	Total O 70 70	0	0
4	D	68	Total O 68 68	0	0
4	E	68	Total O 68 68	0	0
4	F	59	Total O 59 59	0	0
4	G	41	Total O 41 41	0	0
4	H	30	Total O 30 30	0	0

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 errors 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.

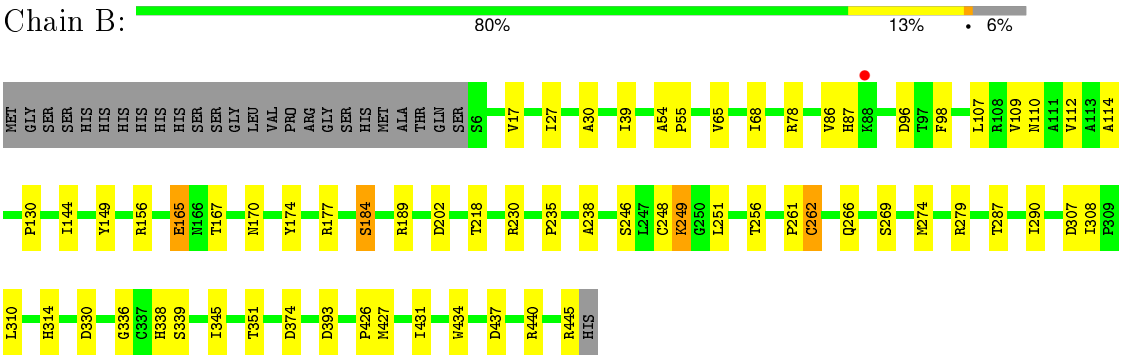
- Molecule 1: Glucarate dehydratase-related protein

Chain A:



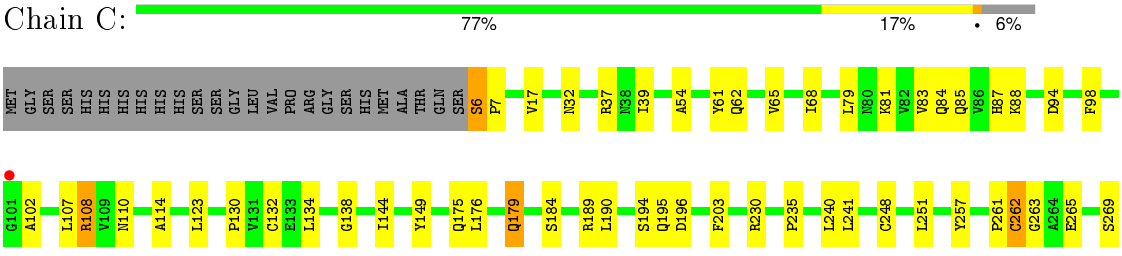
- Molecule 1: Glucarate dehydratase-related protein

Chain B:



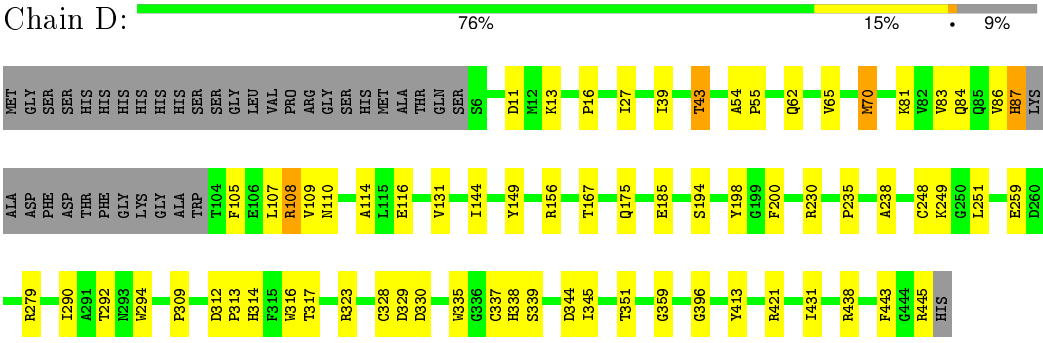
- Molecule 1: Glucarate dehydratase-related protein

Chain C:



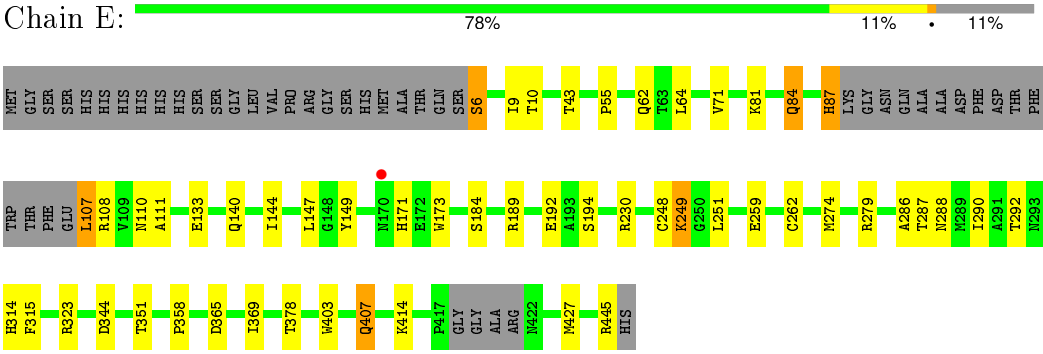
• Molecule 1: Glucarate dehydratase-related protein

Chain D:



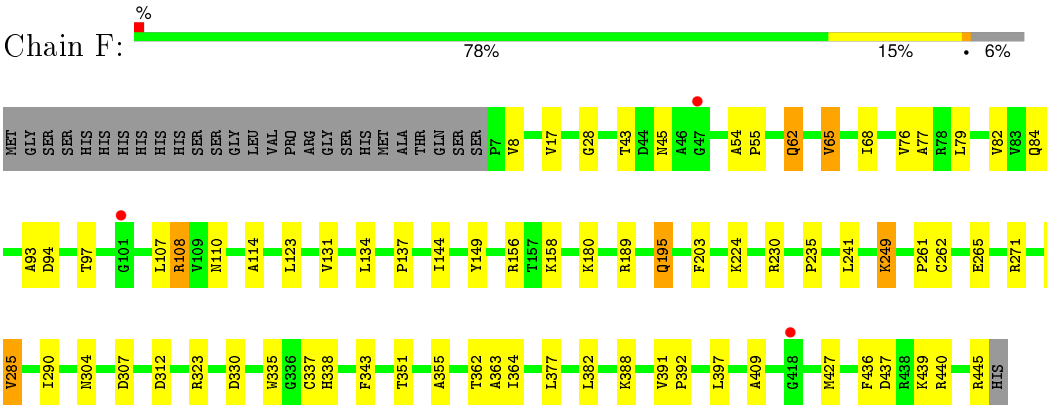
• Molecule 1: Glucarate dehydratase-related protein

Chain E:



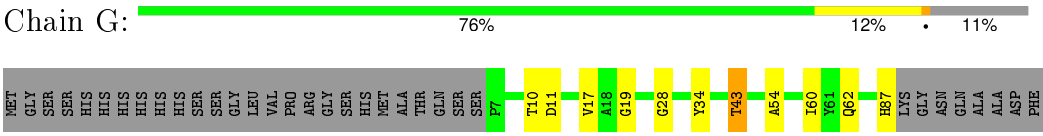
• Molecule 1: Glucarate dehydratase-related protein

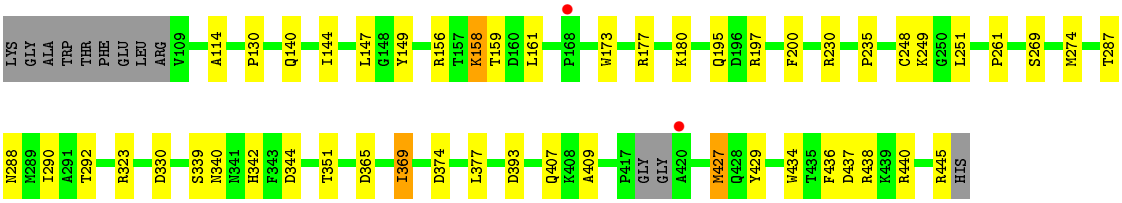
Chain F:



• Molecule 1: Glucarate dehydratase-related protein

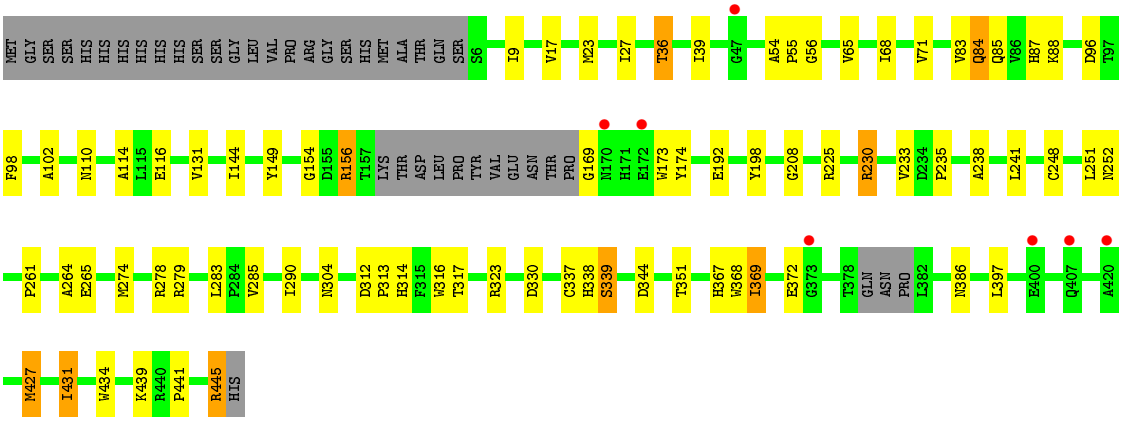
Chain G:





- Molecule 1: Glucarate dehydratase-related protein

Chain H:



4 Data and refinement statistics (i)

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) 91.6 (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 (phenix.refine: 1.8_1066)	Depositor
R, R_{free}	0.173 , 0.231 0.171 , 0.231	Depositor DCC
R_{free} test set	5608 reflections (5.00%)	DCC
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 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 112206 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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:HH11	1:A:189:ARG:HG3	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:B:167:THR:HG23	1:B:174:TYR:HB3	1.77	0.66
1:A:249:LYS:HA	4:A:610:HOH:O	1.94	0.66
1:A:344:ASP:OD2	1:A:378:THR:OG1	2.11	0.66
1:H:431:ILE:O	1:H:431:ILE:HG13	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

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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: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:A:87:HIS:ND1	1:A:87:HIS:O	2.37	0.56
1:H:368:TRP:NE1	1:H:372:GLU:OE1	2.39	0.56
1:C:235:PRO:HG2	1:C:261:PRO:HA	1.87	0.56
1:A:54:ALA:HB2	1:A:114:ALA:HB2	1.86	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:330:ASP:OD2	1:D:323:ARG:NH2	2.40	0.54
1:C:175:GLN:HG2	1:E:403:TRP:CE2	2.42	0.54
1:E:287:THR:OG1	1:E:290:ILE:HG12	2.06	0.54
1:F:271:ARG:HA	1:F:290:ILE:HD12	1.89	0.54
1:E:9:ILE:HG21	1:E:71:VAL:HG12	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:H:278:ARG:NH1	1:H:304:ASN:OD1	2.40	0.53
1:C:84:GLN:HG3	1:C:88:LYS:HZ2	1.73	0.53

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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:B:30:ALA:HB3	1:B:426:PRO:HB2	1.91	0.53
1:A:156:ARG:HG2	4:A:633:HOH:O	2.07	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:F:84:GLN:NE2	1:F:88:LYS:HE2	2.23	0.52
1:A:144:ILE:HD13	1:A:351:THR:HA	1.90	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:H:248:CYS:HA	1:H:251:LEU:HD12	1.93	0.51
1:D:248:CYS:HA	1:D:251:LEU:HD12	1.92	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:F:278:ARG:HG3	1:F:285:VAL:HG13	1.94	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:D:108:ARG:HH11	1:D:108:ARG:HG3	1.76	0.50
1:E:84:GLN:O	1:E:87:HIS:HB3	2.11	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:431:ILE:HD11	1:D:443:PHE:CE1	2.46	0.50
1:A:171:HIS:CD2	1:A:197:ARG:HD3	2.47	0.50
1:H:427:MET:HG3	1:H:434:TRP:CD2	2.47	0.50
1:H:169:GLY:HA3	1:H:174:TYR:HD2	1.76	0.50
1:H:110:ASN:HA	1:H:314:HIS:O	2.12	0.50
1:H:274:MET:HE2	1:H:285:VAL:HG21	1.94	0.50
1:F:93:ALA:O	1:F:97:THR:HG23	2.11	0.50

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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:171:HIS:ND1	3:E:502:GOL:H11	2.26	0.49
1:E:107:LEU:HD13	1:E:315:PHE:HE1	1.77	0.49
1:D:110:ASN:HA	1:D:314:HIS:O	2.12	0.49
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.76	0.49
1:B:230:ARG:N	1:B:230:ARG:HD2	2.26	0.49
1:A:330:ASP:OD2	1:F:323:ARG:NH2	2.46	0.49
1:C:130:PRO:HG3	1:C:393:ASP:HA	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:A:294:TRP:HB3	1:F:330:ASP:HB3	1.94	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:H:173:TRP:CZ2	1:H:369:ILE:HG23	2.48	0.48
1:C:274:MET:HG3	1:C:290:ILE:HD13	1.95	0.48
1:A:316:TRP:O	1:A:317:THR:OG1	2.25	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:C:94:ASP:OD1	1:C:108:ARG:HG3	2.13	0.48
1:B:39:ILE:HD12	1:B:345:ILE:HD12	1.95	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:D:131:VAL:HG23	1:D:396:GLY:C	2.34	0.48
1:A:38:ASN:OD1	1:A:56:GLY:HA2	2.14	0.48
1:D:55:PRO:HD2	1:D:110:ASN:HB3	1.96	0.48
1:F:343:PHE:CD1	1:F:377:LEU:HG	2.49	0.47
1:A:96:ASP:O	1:A:100:LYS:HG3	2.13	0.47
1:A:269:SER:HB3	1:B:269:SER:HB3	1.95	0.47
1:F:55:PRO:HD2	1:F:110:ASN:HB3	1.95	0.47
1:C:437:ASP:HB3	1:C:440:ARG:HB3	1.96	0.47
1:B:27:ILE:HD12	1:B:238:ALA:HB2	1.97	0.47
1:G:28:GLY:HA2	1:G:436:PHE:CD1	2.50	0.47
1:A:261:PRO:HD2	1:A:274:MET:CE	2.44	0.47
1:A:9:ILE:HD11	1:A:71:VAL:O	2.13	0.47
1:G:159:THR:HG22	1:G:429:TYR:CB	2.45	0.47
1:G:11:ASP:HB3	1:G:43:THR:HG22	1.96	0.47

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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:C:175:GLN:HG2	1:E:403:TRP:CD2	2.49	0.47
1:B:86:VAL:HG12	1:B:112:VAL:HG22	1.96	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
1:F:261:PRO:HD2	1:F:274:MET:HE1	1.96	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:A:96:ASP:OD1	1:B:266:GLN:NE2	2.47	0.47
1:C:196:ASP:OD1	1:E:414:LYS:NZ	2.33	0.47
1:C:39:ILE:HD12	1:C:345:ILE:HD12	1.97	0.47
1:H:235:PRO:HG2	1:H:261:PRO:HA	1.97	0.46
1:G:140:GLN:OE1	1:H:84:GLN:NE2	2.48	0.46
1:D:292:THR:HA	4:D:601:HOH:O	2.15	0.46
1:A:84:GLN:HG3	1:F:137:PRO:HB2	1.96	0.46
1:G:173:TRP:CZ2	1:G:369:ILE:HG13	2.51	0.46
1:B:130:PRO:HG3	1:B:393:ASP:HA	1.96	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:D:335:TRP:CH2	1:D:337:CYS:HB2	2.51	0.46
1:A:127:LEU:HD22	1:F:77:ALA:HB2	1.97	0.46
1:C:241:LEU:N	1:C:265:GLU:OE2	2.47	0.46
1:B:54:ALA:HB2	1:B:114:ALA:HB2	1.98	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:H:278:ARG:HG3	1:H:285:VAL:HG13	1.98	0.46
1:C:6:SER:N	1:C:7:PRO:CD	2.78	0.46
1:B:287:THR:HG22	1:B:290:ILE:HD11	1.98	0.45
1:A:9:ILE:HD12	1:A:71:VAL:HG12	1.97	0.45
1:H:85:GLN:HG2	1:H:88:LYS:HD3	1.98	0.45
1:B:78:ARG:NH1	1:E:133:GLU:OE2	2.48	0.45
1:C:343:PHE:CD1	1:C:377:LEU:HG	2.51	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:H:241:LEU:N	1:H:265:GLU:OE2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:ASP:OD1	1:D:359:GLY:HA3	2.15	0.45
1:H:98:PHE:HA	1:H:102:ALA:HB3	1.97	0.45
1:C:263:GLY:H	1:C:439:LYS:HZ3	1.65	0.45
1:A:42:LEU:HD11	1:A:115:LEU:HD12	1.99	0.45
1:E:248:CYS:HA	1:E:251:LEU:HD12	1.97	0.45
1:C:382:LEU:HG	4:C:616:HOH:O	2.16	0.45
1:B:96:ASP:O	4:B:646:HOH:O	2.21	0.45
1:F:355:ALA:HB2	1:F:391:VAL:HG21	1.98	0.45
1:B:65:VAL:HA	1:B:68:ILE:HD12	1.99	0.45
1:H:344:ASP:N	1:H:344:ASP:OD1	2.38	0.45
1:C:179:GLN:HB3	1:C:179:GLN:HE21	1.44	0.45
1:H:96:ASP:O	4:H:625:HOH:O	2.21	0.45
1:B:184:SER:OG	1:B:218:THR:HA	2.17	0.45
1:G:248:CYS:HA	1:G:251:LEU:HD12	1.99	0.45
1:D:83:VAL:HG21	1:D:116:GLU:HG3	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:D:235:PRO:HD2	1:D:259:GLU:O	2.17	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:F:337:CYS:HB3	1:F:364:ILE:HG12	1.98	0.44
1:C:248:CYS:HA	1:C:251:LEU:HD12	1.99	0.44
1:A:234:ASP:HB2	1:A:259:GLU:HB3	1.99	0.44
1:C:110:ASN:HA	1:C:314:HIS:O	2.17	0.44
1:A:61:TYR:O	1:A:65:VAL:HG13	2.18	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:C:84:GLN:CG	1:C:88:LYS:HZ2	2.30	0.44
1:B:310:LEU:HD22	1:B:336:GLY:HA3	2.00	0.44
1:C:312:ASP:HB2	1:C:338:HIS:HB3	2.00	0.44
1:A:195:GLN:HB2	1:A:203:PHE:HZ	1.82	0.44
1:C:176:LEU:HD23	1:C:176:LEU:HA	1.86	0.44
1:E:173:TRP:CZ2	1:E:369:ILE:HG13	2.53	0.44
1:H:65:VAL:HA	1:H:68:ILE:HD12	2.00	0.44
1:B:279:ARG:NH2	1:F:304:ASN:OD1	2.51	0.44
1:G:147:LEU:HD11	1:G:365:ASP:HA	1.99	0.43
1:D:81:LYS:HE3	4:D:620:HOH:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:TYR:CE2	1:H:369:ILE:HD12	2.53	0.43
1:G:200:PHE:CZ	1:G:369:ILE:HG21	2.52	0.43
1:E:140:GLN:HG3	1:E:358:PRO:HA	2.01	0.43
1:A:337:CYS:HB3	1:A:364:ILE:HG23	2.01	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:F:65:VAL:HA	1:F:68:ILE:HD12	2.01	0.42
1:F:8:VAL:HB	1:F:45:ASN:ND2	2.35	0.42
1:C:410:HIS:O	1:C:414:LYS:HG3	2.19	0.42
1:F:312:ASP:HB2	1:F:338:HIS:HB3	2.01	0.42
1:F:28:GLY:HA2	1:F:436:PHE:CD1	2.55	0.42
1:C:333:LEU:HA	1:C:333:LEU:HD23	1.84	0.42
1:F:224:LYS:HB3	1:F:224:LYS:HE3	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:H:23:MET:SD	1:H:154:GLY:HA3	2.60	0.42
1:G:19:GLY:O	1:G:34:TYR:HA	2.19	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:H:84:GLN:HG3	1:H:85:GLN:N	2.34	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:283:LEU:HA	1:H:283:LEU:HD23	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:315:PHE:HZ	1:A:340:ASN:ND2	2.19	0.41
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.85	0.41
1:E:144:ILE:HD13	1:E:351:THR:HA	2.02	0.41
1:E:55:PRO:HD2	1:E:110:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ASP:HB3	1:B:440:ARG:HB3	2.02	0.41
1:D:316:TRP:O	1:D:317:THR:OG1	2.27	0.41
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.93	0.41
1:E:189:ARG:HD3	1:E:192:GLU:OE1	2.21	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:B:307:ASP:C	1:B:308:ILE:HG13	2.40	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:G:197:ARG:O	1:G:197:ARG:HD2	2.21	0.41
1:C:195:GLN:HB2	1:C:203:PHE:HZ	1.86	0.41
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.81	0.41
1:H:251:LEU:HD23	1:H:251:LEU:HA	1.82	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:B:235:PRO:HG2	1:B:261:PRO:HA	2.03	0.41
1:A:94:ASP:OD1	1:A:108:ARG:NH1	2.47	0.41
1:D:344:ASP:N	1:D:344:ASP:OD1	2.44	0.41
1:C:79:LEU:O	1:C:83:VAL:HG23	2.20	0.41
1:A:260:ASP:HA	1:A:274:MET:HE2	2.03	0.40
1:F:107:LEU:O	1:F:110:ASN:ND2	2.53	0.40
1:B:431:ILE:HB	1:B:434:TRP:HB2	2.03	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:HD12	1:G:161:LEU:N	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:O2	2:G:501:CIT:H42	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 (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	438/466 (94%)	429 (98%)	8 (2%)	1 (0%)	52 84
1	B	438/466 (94%)	427 (98%)	10 (2%)	1 (0%)	52 84
1	C	438/466 (94%)	429 (98%)	9 (2%)	0	100 100
1	D	420/466 (90%)	409 (97%)	10 (2%)	1 (0%)	52 84
1	E	411/466 (88%)	405 (98%)	6 (2%)	0	100 100
1	F	437/466 (94%)	431 (99%)	5 (1%)	1 (0%)	52 84
1	G	410/466 (88%)	401 (98%)	8 (2%)	1 (0%)	52 84
1	H	420/466 (90%)	415 (99%)	4 (1%)	1 (0%)	52 84
All	All	3412/3728 (92%)	3346 (98%)	60 (2%)	6 (0%)	52 84

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 (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	350/372 (94%)	332 (95%)	18 (5%)	29 63
1	B	350/372 (94%)	339 (97%)	11 (3%)	47 81
1	C	350/372 (94%)	338 (97%)	12 (3%)	44 78
1	D	340/372 (91%)	323 (95%)	17 (5%)	30 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	336/372 (90%)	319 (95%)	17 (5%)	29 63
1	F	349/372 (94%)	331 (95%)	18 (5%)	29 62
1	G	334/372 (90%)	319 (96%)	15 (4%)	34 68
1	H	336/372 (90%)	322 (96%)	14 (4%)	36 71
All	All	2745/2976 (92%)	2623 (96%)	122 (4%)	35 69

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

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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

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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

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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

Some 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	A	501	-	3,12,12	1.03	0	3,17,17	3.15	3 (100%)
2	CIT	B	501	-	3,12,12	1.29	0	3,17,17	2.02	1 (33%)
2	CIT	C	501	-	3,12,12	1.25	0	3,17,17	3.70	3 (100%)
2	CIT	D	501	-	3,12,12	1.02	0	3,17,17	1.80	1 (33%)
2	CIT	E	501	-	3,12,12	1.11	0	3,17,17	2.20	1 (33%)
3	GOL	E	502	-	5,5,5	0.33	0	5,5,5	0.37	0
2	CIT	F	501	-	3,12,12	1.46	1 (33%)	3,17,17	1.71	1 (33%)
2	CIT	G	501	-	3,12,12	1.30	0	3,17,17	3.12	2 (66%)
3	GOL	G	502	-	5,5,5	0.26	0	5,5,5	0.64	0
2	CIT	H	501	-	3,12,12	1.03	0	3,17,17	1.00	0

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	A	501	-	-	0/6/16/16	0/0/0/0
2	CIT	B	501	-	-	0/6/16/16	0/0/0/0
2	CIT	C	501	-	-	0/6/16/16	0/0/0/0
2	CIT	D	501	-	-	0/6/16/16	0/0/0/0
2	CIT	E	501	-	-	0/6/16/16	0/0/0/0
3	GOL	E	502	-	-	0/4/4/4	0/0/0/0
2	CIT	F	501	-	-	0/6/16/16	0/0/0/0
2	CIT	G	501	-	-	0/6/16/16	0/0/0/0
3	GOL	G	502	-	-	0/4/4/4	0/0/0/0
2	CIT	H	501	-	-	0/6/16/16	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	CIT	O7-C3	2.07	1.46	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	501	CIT	C3-C4-C5	-4.76	107.35	114.96
2	C	501	CIT	C3-C4-C5	-4.26	108.14	114.96
2	E	501	CIT	C3-C4-C5	-3.29	109.70	114.96
2	B	501	CIT	C3-C4-C5	-3.14	109.93	114.96
2	D	501	CIT	C3-C4-C5	-2.89	110.34	114.96
2	F	501	CIT	C3-C4-C5	-2.23	111.39	114.96
2	A	501	CIT	C3-C2-C1	-2.12	111.56	114.96
2	A	501	CIT	C3-C4-C5	2.15	118.40	114.96
2	G	501	CIT	C4-C3-C2	2.57	115.94	109.81
2	C	501	CIT	C3-C2-C1	3.25	120.15	114.96
2	C	501	CIT	C4-C3-C2	3.52	118.22	109.81
2	A	501	CIT	C4-C3-C2	4.53	120.65	109.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	440/466 (94%)	-0.65	6 (1%) 78 69	8, 21, 58, 98	0
1	B	440/466 (94%)	-0.74	1 (0%) 95 94	10, 22, 45, 70	0
1	C	440/466 (94%)	-0.76	1 (0%) 95 94	10, 20, 42, 82	0
1	D	424/466 (90%)	-0.74	0 100 100	11, 23, 40, 73	0
1	E	417/466 (89%)	-0.76	1 (0%) 95 94	9, 21, 37, 58	0
1	F	439/466 (94%)	-0.63	3 (0%) 89 84	9, 28, 53, 66	0
1	G	416/466 (89%)	-0.67	2 (0%) 91 88	12, 28, 45, 66	0
1	H	426/466 (91%)	-0.42	7 (1%) 74 66	13, 39, 61, 93	0
All	All	3442/3728 (92%)	-0.67	21 (0%) 90 86	8, 24, 53, 98	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	ASN	3.7
1	F	47	GLY	3.1
1	G	420	ALA	3.0
1	A	88	LYS	2.8
1	H	373	GLY	2.8
1	A	47	GLY	2.8
1	H	170	ASN	2.7
1	C	101	GLY	2.7
1	H	407	GLN	2.7
1	H	172	GLU	2.6
1	A	92	ALA	2.6
1	A	97	THR	2.5
1	H	420	ALA	2.3
1	F	101	GLY	2.2
1	H	400	GLU	2.1
1	A	96	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	168	PRO	2.1
1	H	47	GLY	2.0
1	E	170	ASN	2.0
1	B	88	LYS	2.0
1	F	418	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CIT	E	501	13/13	0.97	0.21	2.94	8,20,36,48	0
2	CIT	D	501	13/13	0.95	0.17	0.62	17,33,48,48	0
2	CIT	G	501	13/13	0.97	0.15	0.49	23,40,46,49	0
2	CIT	B	501	13/13	0.98	0.13	0.20	16,24,30,33	0
2	CIT	A	501	13/13	0.97	0.14	-0.02	27,31,43,57	0
2	CIT	F	501	13/13	0.97	0.13	-0.04	22,31,43,45	0
2	CIT	H	501	13/13	0.97	0.12	-0.54	30,39,49,59	0
2	CIT	C	501	13/13	0.97	0.11	-0.59	11,22,31,45	0
3	GOL	G	502	6/6	0.83	0.16	-	27,33,40,41	0
3	GOL	E	502	6/6	0.94	0.13	-	6,21,33,35	0

6.5 Other polymers (i)

There are no such residues in this entry.