



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:08 AM GMT

PDB ID : 3SOM
Title : crystal structure of human MMACHC
Authors : Krojer, T.; Froese, D.S.; von Delft, F.; Muniz, J.R.; Gileadi, C.; Vollmar, M.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Gravel, R.A.; Yue, W.W.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2011-06-30
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

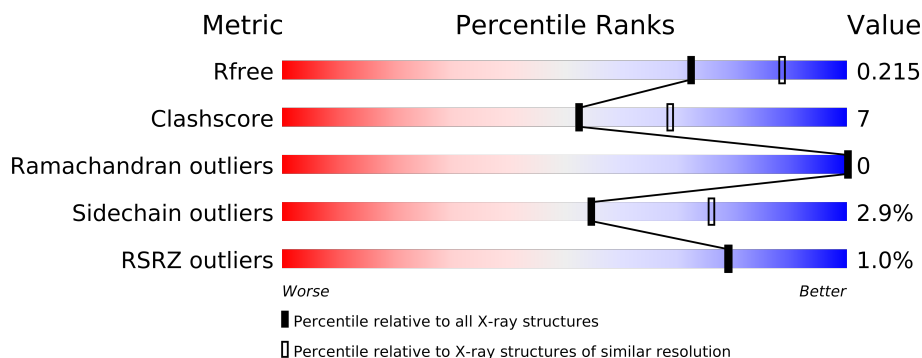
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	
1	C	286	
1	D	286	
1	E	286	
1	F	286	
1	G	286	
1	H	286	
1	I	286	
1	J	286	
1	K	286	
1	L	286	
1	M	286	
1	N	286	

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Mol	Chain	Length	Quality of chain
1	O	286	
1	P	286	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	FLC	B	501	-	X
4	DHL	A	601	-	X
4	DHL	D	601	-	X
4	DHL	G	601	-	X
4	DHL	I	601	-	X
4	DHL	J	601	-	X
4	DHL	K	601	-	X
4	DHL	M	601	-	X
4	DHL	N	601	-	X
4	DHL	O	601	-	X
5	5AD	B	401	-	X
5	5AD	D	401	-	X
5	5AD	G	283	-	X
5	5AD	H	401	-	X
5	5AD	I	283	-	X
5	5AD	M	401	-	X
6	EDO	E	283	-	X
6	EDO	P	283	-	X
6	EDO	P	284	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33236 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Methylmalonic aciduria and homocystinuria type C protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	Se	0	0	0
			1837	1193	319	318	5	2			
1	B	228	Total	C	N	O	S	Se	0	0	0
			1837	1193	319	318	5	2			
1	C	228	Total	C	N	O	S	Se	0	2	0
			1832	1190	318	316	6	2			
1	D	229	Total	C	N	O	S	Se	0	1	0
			1848	1200	320	320	6	2			
1	E	230	Total	C	N	O	S	Se	0	1	0
			1849	1201	321	319	6	2			
1	F	228	Total	C	N	O	S	Se	0	3	0
			1857	1203	324	322	6	2			
1	G	228	Total	C	N	O	S	Se	0	0	0
			1843	1195	322	319	5	2			
1	H	227	Total	C	N	O	S	Se	0	0	0
			1833	1190	317	319	5	2			
1	I	228	Total	C	N	O	S	Se	0	1	0
			1844	1196	321	319	6	2			
1	J	227	Total	C	N	O	S	Se	0	2	0
			1844	1196	321	319	5	3			
1	K	227	Total	C	N	O	S	Se	0	1	0
			1832	1189	318	318	5	2			
1	L	231	Total	C	N	O	S	Se	0	2	0
			1868	1213	325	322	6	2			
1	M	231	Total	C	N	O	S	Se	0	1	0
			1861	1206	321	326	6	2			
1	N	232	Total	C	N	O	S	Se	0	0	0
			1853	1204	324	318	5	2			
1	O	228	Total	C	N	O	S	Se	0	1	0
			1836	1194	316	318	6	2			
1	P	230	Total	C	N	O	S	Se	0	0	0
			1860	1208	322	323	5	2			

There are 64 discrepancies between the modelled and reference sequences:

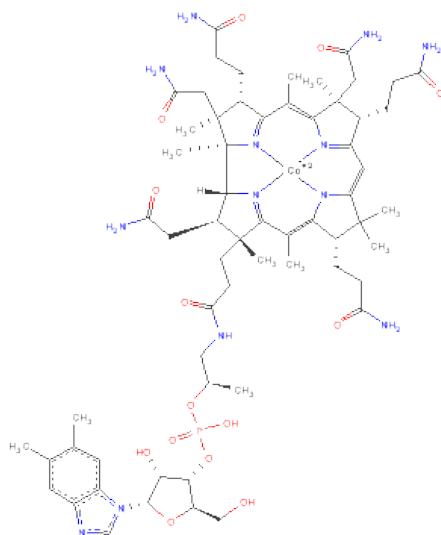
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
A	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
A	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
A	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
B	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
B	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
B	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
B	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
C	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
C	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
C	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
C	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
D	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
D	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
D	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
D	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
E	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
E	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
E	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
E	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
F	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
F	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
F	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
F	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
G	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
G	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
G	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
G	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
H	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
H	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
H	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
H	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
I	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
I	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
I	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
I	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
J	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
J	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
J	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
J	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
K	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
K	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1

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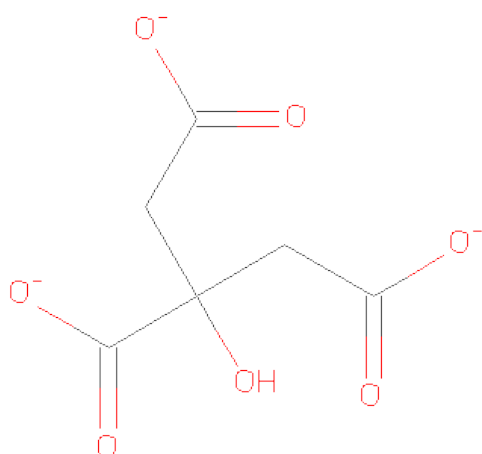
Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
K	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
L	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
L	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
L	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
L	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
M	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
M	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
M	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
M	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
N	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
N	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
N	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
N	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
O	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
O	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
O	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
O	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
P	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
P	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
P	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
P	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	E	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	F	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	G	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	H	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	I	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	J	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	K	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	L	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	M	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	N	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	O	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
2	P	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $\text{C}_6\text{H}_5\text{O}_7$).



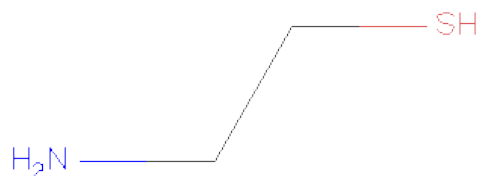
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		
3	H	1	Total	C	O	0	0
			13	6	7		
3	I	1	Total	C	O	0	0
			13	6	7		
3	J	1	Total	C	O	0	0
			13	6	7		
3	K	1	Total	C	O	0	0
			13	6	7		
3	L	1	Total	C	O	0	0
			13	6	7		
3	M	1	Total	C	O	0	0
			13	6	7		
3	N	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			13	6	7		
3	P	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 2-AMINO-ETHANETHIOL (three-letter code: DHL) (formula: C₂H₇NS).



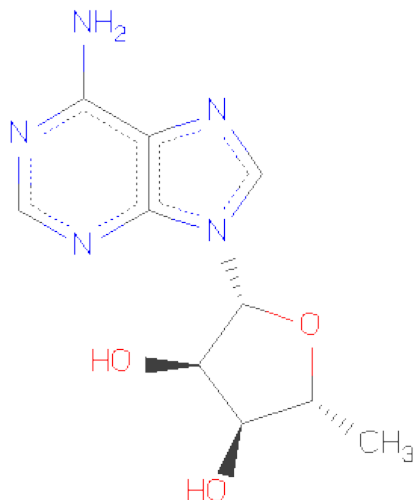
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			4	2	1	1		
4	C	1	Total	C	N	S	0	0
			4	2	1	1		
4	D	1	Total	C	N	S	0	0
			4	2	1	1		
4	F	1	Total	C	N	S	0	0
			4	2	1	1		
4	G	1	Total	C	N	S	0	0
			4	2	1	1		
4	H	1	Total	C	N	S	0	0
			4	2	1	1		
4	I	1	Total	C	N	S	0	0
			4	2	1	1		
4	J	1	Total	C	N	S	0	0
			4	2	1	1		
4	K	1	Total	C	N	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	S	0	0
			4	2	1	1		
4	M	1	Total	C	N	S	0	0
			4	2	1	1		
4	N	1	Total	C	N	S	0	0
			4	2	1	1		
4	O	1	Total	C	N	S	0	0
			4	2	1	1		
4	P	1	Total	C	N	S	0	0
			4	2	1	1		

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: C₁₀H₁₃N₅O₃).



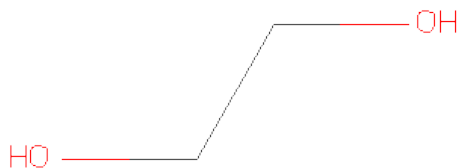
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		
5	C	1	Total	C	N	O	0	0
			18	10	5	3		
5	D	1	Total	C	N	O	0	0
			18	10	5	3		
5	E	1	Total	C	N	O	0	0
			18	10	5	3		
5	F	1	Total	C	N	O	0	0
			18	10	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			18	10	5	3		
5	G	1	Total	C	N	O	0	0
			18	10	5	3		
5	H	1	Total	C	N	O	0	0
			18	10	5	3		
5	I	1	Total	C	N	O	0	0
			18	10	5	3		
5	I	1	Total	C	N	O	0	0
			18	10	5	3		
5	J	1	Total	C	N	O	0	0
			18	10	5	3		
5	K	1	Total	C	N	O	0	0
			18	10	5	3		
5	L	1	Total	C	N	O	0	0
			18	10	5	3		
5	M	1	Total	C	N	O	0	0
			18	10	5	3		
5	N	1	Total	C	N	O	0	0
			18	10	5	3		
5	O	1	Total	C	N	O	0	0
			18	10	5	3		
5	P	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

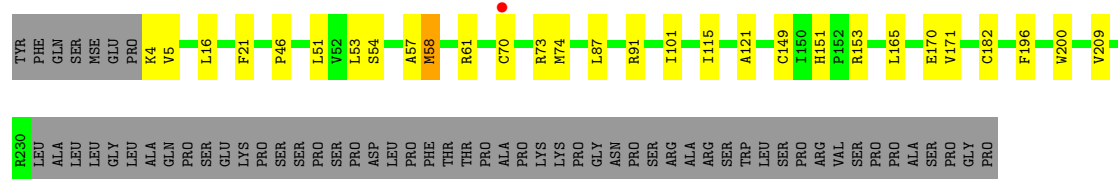


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 4 2 2	0	0
6	P	1	Total C O 4 2 2	0	0
6	P	1	Total C O 4 2 2	0	0

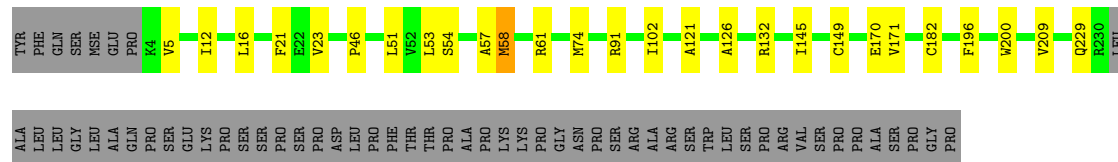
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	63	Total O 63 63	0	0
7	C	63	Total O 63 63	0	0
7	D	79	Total O 79 79	0	0
7	E	105	Total O 105 105	0	0
7	F	111	Total O 111 111	0	0
7	G	125	Total O 125 125	0	0
7	H	124	Total O 124 124	0	0
7	I	122	Total O 122 122	0	0
7	J	111	Total O 111 111	0	0
7	K	100	Total O 100 100	0	0
7	L	130	Total O 130 130	0	0
7	M	125	Total O 125 125	0	0
7	N	100	Total O 100 100	0	0
7	O	124	Total O 124 124	0	0
7	P	94	Total O 94 94	0	0

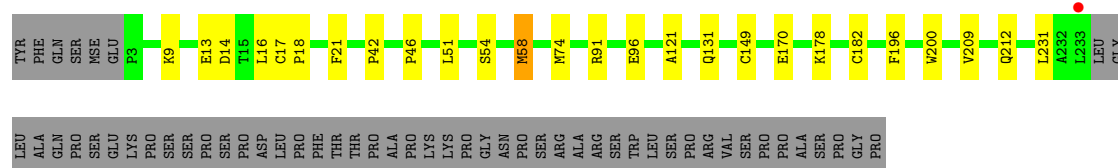


Chain J: 

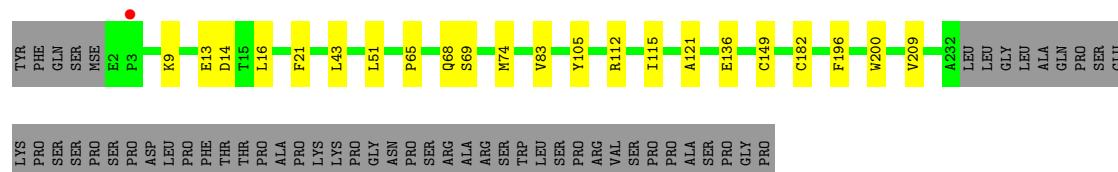
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain K: 

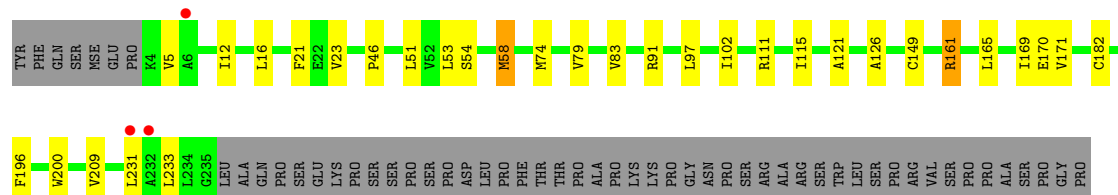
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain L: 

- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

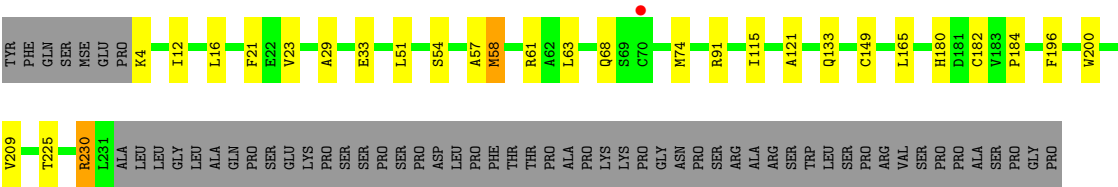
Chain M: 

- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain N: 

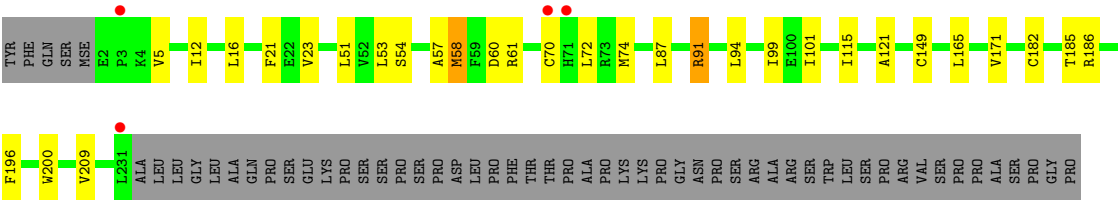
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain O: 



● Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.66Å 71.96Å 300.06Å 88.53° 85.25° 83.76°	Depositor
Resolution (Å)	19.86 – 2.40 19.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.86-2.40) 98.7 (19.84-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.41Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.182 , 0.206 0.190 , 0.215	Depositor DCC
R_{free} test set	11473 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.8	EDS
Estimated twinning fraction	0.007 for -h,-k,-h+l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 228734 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33236	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, DHL, B12, EDO, 5AD

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	0.47	0/1898	0.63	0/2592
1	B	0.45	0/1899	0.64	0/2595
1	C	0.46	0/1899	0.64	0/2598
1	D	0.47	0/1913	0.64	0/2616
1	E	0.47	0/1913	0.65	0/2615
1	F	0.50	0/1928	0.67	0/2635
1	G	0.48	0/1905	0.64	0/2603
1	H	0.48	0/1894	0.65	0/2588
1	I	0.46	0/1909	0.64	0/2609
1	J	0.48	0/1911	0.66	0/2610
1	K	0.49	0/1899	0.66	0/2596
1	L	0.49	0/1936	0.68	0/2646
1	M	0.49	0/1926	0.66	0/2635
1	N	0.48	0/1914	0.67	0/2618
1	O	0.49	0/1900	0.67	0/2596
1	P	0.48	0/1922	0.65	0/2626
All	All	0.48	0/30566	0.65	0/41778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1837	0	1791	15	0
1	B	1837	0	1792	15	0
1	C	1832	0	1779	18	0
1	D	1848	0	1798	20	0
1	E	1849	0	1802	18	0
1	F	1857	0	1813	19	0
1	G	1843	0	1797	21	0
1	H	1833	0	1782	22	0
1	I	1844	0	1796	22	0
1	J	1844	0	1804	16	0
1	K	1832	0	1783	21	0
1	L	1868	0	1826	17	0
1	M	1861	0	1800	19	0
1	N	1853	0	1806	21	0
1	O	1836	0	1786	23	0
1	P	1860	0	1817	22	0
2	A	91	0	88	14	0
2	B	91	0	88	13	0
2	C	91	0	88	15	0
2	D	91	0	88	12	0
2	E	91	0	88	14	0
2	F	91	0	88	13	0
2	G	91	0	88	15	0
2	H	91	0	88	13	0
2	I	91	0	88	14	0
2	J	91	0	88	12	0
2	K	91	0	88	12	0
2	L	91	0	88	13	0
2	M	91	0	88	12	0
2	N	91	0	88	13	0
2	O	91	0	88	15	0
2	P	91	0	88	16	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	0	0
3	F	13	0	5	0	0
3	G	13	0	5	0	0
3	H	13	0	5	0	0
3	I	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	13	0	5	0	0
3	K	13	0	5	0	0
3	L	13	0	5	0	0
3	M	13	0	5	0	0
3	N	13	0	5	0	0
3	O	13	0	5	0	0
3	P	13	0	5	0	0
4	A	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	2	0
4	F	4	0	6	0	0
4	G	4	0	6	1	0
4	H	4	0	6	0	0
4	I	4	0	7	3	0
4	J	4	0	7	1	0
4	K	4	0	7	3	0
4	L	4	0	6	0	0
4	M	4	0	6	0	0
4	N	4	0	7	1	0
4	O	4	0	6	1	0
4	P	4	0	6	0	0
5	A	18	0	13	3	0
5	B	18	0	13	3	0
5	C	18	0	13	4	0
5	D	18	0	13	3	0
5	E	18	0	13	3	0
5	F	18	0	13	3	0
5	G	36	0	26	4	0
5	H	18	0	13	4	0
5	I	36	0	26	4	0
5	J	18	0	13	3	0
5	K	18	0	13	3	0
5	L	18	0	13	3	0
5	M	18	0	13	3	0
5	N	18	0	13	4	0
5	O	18	0	13	3	0
5	P	18	0	13	3	0
6	E	4	0	6	2	0
6	P	8	0	12	7	0
7	A	70	0	0	0	0
7	B	63	0	0	1	0
7	C	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	79	0	0	0	0
7	E	105	0	0	0	0
7	F	111	0	0	0	0
7	G	125	0	0	1	0
7	H	124	0	0	0	0
7	I	122	0	0	2	0
7	J	111	0	0	0	0
7	K	100	0	0	0	0
7	L	130	0	0	0	0
7	M	125	0	0	3	0
7	N	100	0	0	0	0
7	O	124	0	0	1	0
7	P	94	0	0	0	0
All	All	33236	0	30600	442	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 442 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:182:CYS:SG	4:D:601:DHL:SG	2.33	1.26
2:A:301:B12:H362	2:A:301:B12:H351	1.37	1.06
2:P:301:B12:H362	2:P:301:B12:H351	1.37	1.05
2:D:301:B12:H362	2:D:301:B12:H351	1.39	1.03
2:O:301:B12:H351	2:O:301:B12:H362	1.40	1.03

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	225/286 (79%)	222 (99%)	3 (1%)	0	100	100
1	B	226/286 (79%)	222 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	228/286 (80%)	226 (99%)	2 (1%)	0	100	100
1	D	228/286 (80%)	224 (98%)	4 (2%)	0	100	100
1	E	229/286 (80%)	227 (99%)	2 (1%)	0	100	100
1	F	229/286 (80%)	225 (98%)	4 (2%)	0	100	100
1	G	226/286 (79%)	223 (99%)	3 (1%)	0	100	100
1	H	225/286 (79%)	224 (100%)	1 (0%)	0	100	100
1	I	227/286 (79%)	223 (98%)	4 (2%)	0	100	100
1	J	227/286 (79%)	224 (99%)	3 (1%)	0	100	100
1	K	226/286 (79%)	224 (99%)	2 (1%)	0	100	100
1	L	231/286 (81%)	228 (99%)	3 (1%)	0	100	100
1	M	230/286 (80%)	228 (99%)	2 (1%)	0	100	100
1	N	230/286 (80%)	229 (100%)	1 (0%)	0	100	100
1	O	227/286 (79%)	224 (99%)	3 (1%)	0	100	100
1	P	228/286 (80%)	227 (100%)	1 (0%)	0	100	100
All	All	3642/4576 (80%)	3600 (99%)	42 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	193/243 (79%)	187 (97%)	6 (3%)	52	74
1	B	193/243 (79%)	187 (97%)	6 (3%)	52	74
1	C	192/243 (79%)	184 (96%)	8 (4%)	40	60
1	D	194/243 (80%)	187 (96%)	7 (4%)	47	68
1	E	193/243 (79%)	187 (97%)	6 (3%)	52	74
1	F	197/243 (81%)	192 (98%)	5 (2%)	60	80
1	G	194/243 (80%)	189 (97%)	5 (3%)	59	79
1	H	192/243 (79%)	186 (97%)	6 (3%)	52	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	194/243 (80%)	189 (97%)	5 (3%)	59	79
1	J	195/243 (80%)	189 (97%)	6 (3%)	52	74
1	K	192/243 (79%)	189 (98%)	3 (2%)	75	89
1	L	196/243 (81%)	190 (97%)	6 (3%)	52	74
1	M	195/243 (80%)	193 (99%)	2 (1%)	85	95
1	N	192/243 (79%)	186 (97%)	6 (3%)	52	74
1	O	192/243 (79%)	185 (96%)	7 (4%)	47	68
1	P	196/243 (81%)	189 (96%)	7 (4%)	47	68
All	All	3100/3888 (80%)	3009 (97%)	91 (3%)	55	76

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	115	ILE
1	I	73	ARG
1	P	53	LEU
1	G	133	GLN
1	H	115	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	131	GLN
1	I	199	HIS
1	M	68	GLN
1	G	131	GLN
1	L	131	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

67 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	B12	A	301	5	101,101,101	9.18	15 (14%)	152,166,166	2.26	21 (13%)
5	5AD	A	401	2	20,20,20	1.26	2 (10%)	30,30,30	2.01	8 (26%)
3	FLC	A	501	-	5,12,12	3.02	2 (40%)	7,17,17	0.68	0
4	DHL	A	601	1	3,3,3	1.33	0	2,2,2	1.00	0
2	B12	B	301	5	101,101,101	8.98	13 (12%)	152,166,166	2.29	23 (15%)
5	5AD	B	401	2	20,20,20	1.31	2 (10%)	30,30,30	2.10	8 (26%)
3	FLC	B	501	-	5,12,12	3.66	2 (40%)	7,17,17	0.60	0
2	B12	C	301	5	101,101,101	8.88	13 (12%)	152,166,166	2.31	22 (14%)
5	5AD	C	401	2	20,20,20	1.30	2 (10%)	30,30,30	2.10	7 (23%)
3	FLC	C	501	-	5,12,12	2.58	2 (40%)	7,17,17	0.58	0
4	DHL	C	601	-	3,3,3	1.16	0	2,2,2	1.34	0
2	B12	D	301	5	101,101,101	9.44	13 (12%)	152,166,166	2.28	21 (13%)
5	5AD	D	401	2	20,20,20	1.23	3 (15%)	30,30,30	2.12	8 (26%)
3	FLC	D	501	-	5,12,12	3.68	3 (60%)	7,17,17	0.89	0
4	DHL	D	601	-	3,3,3	1.69	1 (33%)	2,2,2	1.13	0
6	EDO	E	283	-	3,3,3	0.60	0	2,2,2	0.17	0
2	B12	E	301	5	101,101,101	8.65	13 (12%)	152,166,166	2.26	21 (13%)
5	5AD	E	401	2	20,20,20	1.28	3 (15%)	30,30,30	2.27	7 (23%)
3	FLC	E	501	-	5,12,12	3.45	2 (40%)	7,17,17	0.88	0
2	B12	F	301	5	101,101,101	8.86	14 (13%)	152,166,166	2.22	19 (12%)
5	5AD	F	401	2	20,20,20	1.29	2 (10%)	30,30,30	2.04	9 (30%)
3	FLC	F	501	-	5,12,12	3.47	2 (40%)	7,17,17	0.94	0
4	DHL	F	601	1	3,3,3	1.43	1 (33%)	2,2,2	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5AD	G	283	-	20,20,20	1.27	4 (20%)	30,30,30	2.28	6 (20%)
2	B12	G	301	5	101,101,101	9.32	14 (13%)	152,166,166	2.23	20 (13%)
5	5AD	G	401	2	20,20,20	1.27	2 (10%)	30,30,30	2.16	8 (26%)
3	FLC	G	501	-	5,12,12	3.42	2 (40%)	7,17,17	0.83	0
4	DHL	G	601	1	3,3,3	1.16	0	2,2,2	2.63	1 (50%)
2	B12	H	301	5	101,101,101	9.50	13 (12%)	152,166,166	2.33	21 (13%)
5	5AD	H	401	2	20,20,20	1.22	2 (10%)	30,30,30	2.18	8 (26%)
3	FLC	H	501	-	5,12,12	2.56	2 (40%)	7,17,17	0.69	0
4	DHL	H	601	1	3,3,3	1.36	1 (33%)	2,2,2	2.39	1 (50%)
5	5AD	I	283	-	20,20,20	1.23	2 (10%)	30,30,30	2.18	7 (23%)
2	B12	I	301	5	101,101,101	9.61	14 (13%)	152,166,166	2.29	22 (14%)
5	5AD	I	401	2	20,20,20	1.31	3 (15%)	30,30,30	2.07	8 (26%)
3	FLC	I	501	-	5,12,12	3.28	2 (40%)	7,17,17	0.72	0
4	DHL	I	601	-	3,3,3	1.38	1 (33%)	2,2,2	3.49	1 (50%)
2	B12	J	301	5	101,101,101	9.16	15 (14%)	152,166,166	2.23	21 (13%)
5	5AD	J	401	2	20,20,20	1.31	3 (15%)	30,30,30	2.11	9 (30%)
3	FLC	J	501	-	5,12,12	3.72	2 (40%)	7,17,17	0.80	0
4	DHL	J	601	-	3,3,3	1.62	1 (33%)	2,2,2	1.40	0
2	B12	K	301	5	101,101,101	8.52	13 (12%)	152,166,166	2.31	21 (13%)
5	5AD	K	401	2	20,20,20	1.35	3 (15%)	30,30,30	2.07	8 (26%)
3	FLC	K	501	-	5,12,12	3.44	2 (40%)	7,17,17	0.77	0
4	DHL	K	601	-	3,3,3	1.69	1 (33%)	2,2,2	0.40	0
2	B12	L	301	5	101,101,101	9.52	14 (13%)	152,166,166	2.29	22 (14%)
5	5AD	L	401	2	20,20,20	1.27	2 (10%)	30,30,30	2.09	8 (26%)
3	FLC	L	501	-	5,12,12	3.50	2 (40%)	7,17,17	0.63	0
4	DHL	L	601	-	3,3,3	1.69	1 (33%)	2,2,2	1.30	0
2	B12	M	301	5	101,101,101	9.12	14 (13%)	152,166,166	2.27	20 (13%)
5	5AD	M	401	2	20,20,20	1.25	2 (10%)	30,30,30	2.07	7 (23%)
3	FLC	M	501	-	5,12,12	3.48	2 (40%)	7,17,17	0.93	0
4	DHL	M	601	-	3,3,3	1.48	1 (33%)	2,2,2	0.61	0
2	B12	N	301	5	101,101,101	8.89	13 (12%)	152,166,166	2.23	21 (13%)
5	5AD	N	401	2	20,20,20	1.23	2 (10%)	30,30,30	2.19	8 (26%)
3	FLC	N	501	-	5,12,12	2.08	2 (40%)	7,17,17	0.64	0
4	DHL	N	601	-	3,3,3	1.73	1 (33%)	2,2,2	1.90	1 (50%)
2	B12	O	301	5	101,101,101	8.96	14 (13%)	152,166,166	2.24	22 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5AD	O	401	2	20,20,20	1.34	2 (10%)	30,30,30	2.06	8 (26%)
3	FLC	O	501	-	5,12,12	3.16	2 (40%)	7,17,17	0.81	0
4	DHL	O	601	1	3,3,3	1.36	1 (33%)	2,2,2	0.66	0
6	EDO	P	283	-	3,3,3	0.63	0	2,2,2	0.14	0
6	EDO	P	284	-	3,3,3	0.49	0	2,2,2	0.18	0
2	B12	P	301	5	101,101,101	9.45	15 (14%)	152,166,166	2.26	22 (14%)
5	5AD	P	401	2	20,20,20	1.25	2 (10%)	30,30,30	2.04	8 (26%)
3	FLC	P	501	-	5,12,12	3.82	2 (40%)	7,17,17	0.71	0
4	DHL	P	601	-	3,3,3	1.19	0	2,2,2	1.05	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	B12	A	301	5	-	0/56/223/223	0/1/11/11
5	5AD	A	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	A	501	-	-	0/6/16/16	0/0/0/0
4	DHL	A	601	1	-	0/1/1/1	0/0/0/0
2	B12	B	301	5	-	0/56/223/223	0/1/11/11
5	5AD	B	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	B	501	-	-	0/6/16/16	0/0/0/0
2	B12	C	301	5	-	0/56/223/223	0/1/11/11
5	5AD	C	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	C	501	-	-	0/6/16/16	0/0/0/0
4	DHL	C	601	-	-	0/1/1/1	0/0/0/0
2	B12	D	301	5	-	0/56/223/223	0/1/11/11
5	5AD	D	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	D	501	-	-	0/6/16/16	0/0/0/0
4	DHL	D	601	-	-	0/1/1/1	0/0/0/0
6	EDO	E	283	-	-	0/1/1/1	0/0/0/0
2	B12	E	301	5	-	0/56/223/223	0/1/11/11
5	5AD	E	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	E	501	-	-	0/6/16/16	0/0/0/0
2	B12	F	301	5	-	0/56/223/223	0/1/11/11
5	5AD	F	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	F	501	-	-	0/6/16/16	0/0/0/0
4	DHL	F	601	1	-	0/1/1/1	0/0/0/0
5	5AD	G	283	-	1/1/4/4	0/4/20/20	0/1/3/3
2	B12	G	301	5	-	0/56/223/223	0/1/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5AD	G	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	G	501	-	-	0/6/16/16	0/0/0/0
4	DHL	G	601	1	-	0/1/1/1	0/0/0/0
2	B12	H	301	5	-	0/56/223/223	0/1/11/11
5	5AD	H	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	H	501	-	-	0/6/16/16	0/0/0/0
4	DHL	H	601	1	-	0/1/1/1	0/0/0/0
5	5AD	I	283	-	1/1/4/4	0/4/20/20	0/1/3/3
2	B12	I	301	5	-	0/56/223/223	0/1/11/11
5	5AD	I	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	I	501	-	-	0/6/16/16	0/0/0/0
4	DHL	I	601	-	-	0/1/1/1	0/0/0/0
2	B12	J	301	5	-	0/56/223/223	0/1/11/11
5	5AD	J	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	J	501	-	-	0/6/16/16	0/0/0/0
4	DHL	J	601	-	-	0/1/1/1	0/0/0/0
2	B12	K	301	5	-	0/56/223/223	0/1/11/11
5	5AD	K	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	K	501	-	-	0/6/16/16	0/0/0/0
4	DHL	K	601	-	-	0/1/1/1	0/0/0/0
2	B12	L	301	5	-	0/56/223/223	0/1/11/11
5	5AD	L	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	L	501	-	-	0/6/16/16	0/0/0/0
4	DHL	L	601	-	-	0/1/1/1	0/0/0/0
2	B12	M	301	5	-	0/56/223/223	0/1/11/11
5	5AD	M	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	M	501	-	-	0/6/16/16	0/0/0/0
4	DHL	M	601	-	-	0/1/1/1	0/0/0/0
2	B12	N	301	5	-	0/56/223/223	0/1/11/11
5	5AD	N	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	N	501	-	-	0/6/16/16	0/0/0/0
4	DHL	N	601	-	-	0/1/1/1	0/0/0/0
2	B12	O	301	5	-	0/56/223/223	0/1/11/11
5	5AD	O	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	O	501	-	-	0/6/16/16	0/0/0/0
4	DHL	O	601	1	-	0/1/1/1	0/0/0/0
6	EDO	P	283	-	-	0/1/1/1	0/0/0/0
6	EDO	P	284	-	-	0/1/1/1	0/0/0/0
2	B12	P	301	5	-	0/56/223/223	0/1/11/11
5	5AD	P	401	2	1/1/4/4	0/4/20/20	0/1/3/3
3	FLC	P	501	-	-	0/6/16/16	0/0/0/0
4	DHL	P	601	-	-	0/1/1/1	0/0/0/0

The worst 5 of 306 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	B12	CO-N24	82.12	1.96	1.79
2	H	301	B12	CO-N24	82.10	1.96	1.79
2	L	301	B12	CO-N24	82.05	1.96	1.79
2	D	301	B12	CO-N24	81.81	1.96	1.79
2	P	301	B12	CO-N24	80.41	1.95	1.79

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	B12	C19-N24-C16	-17.14	99.92	109.08
2	L	301	B12	C19-N24-C16	-16.94	100.03	109.08
2	I	301	B12	C19-N24-C16	-16.79	100.11	109.08
2	B	301	B12	C19-N24-C16	-16.76	100.13	109.08
2	C	301	B12	C19-N24-C16	-16.71	100.15	109.08

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	I	401	5AD	C4'
5	M	401	5AD	C4'
5	J	401	5AD	C4'
5	G	401	5AD	C4'
5	K	401	5AD	C4'

There are no torsion outliers.

There are no ring outliers.

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	227/286 (79%)	-0.28	4 (1%) 65 63	24, 40, 58, 70	0
1	B	228/286 (79%)	-0.23	3 (1%) 74 73	26, 40, 60, 70	0
1	C	228/286 (79%)	-0.05	5 (2%) 59 57	29, 43, 60, 76	0
1	D	229/286 (80%)	-0.36	3 (1%) 74 73	23, 35, 52, 73	0
1	E	230/286 (80%)	-0.45	2 (0%) 81 81	18, 31, 51, 72	0
1	F	228/286 (79%)	-0.51	0 100 100	16, 29, 47, 63	0
1	G	228/286 (79%)	-0.52	3 (1%) 74 73	16, 27, 48, 68	0
1	H	227/286 (79%)	-0.56	2 (0%) 81 81	17, 27, 47, 66	0
1	I	228/286 (79%)	-0.49	2 (0%) 81 81	19, 30, 52, 71	0
1	J	227/286 (79%)	-0.53	1 (0%) 90 90	19, 29, 50, 71	0
1	K	227/286 (79%)	-0.44	0 100 100	19, 32, 51, 67	0
1	L	231/286 (80%)	-0.52	1 (0%) 90 90	16, 28, 45, 71	0
1	M	231/286 (80%)	-0.50	1 (0%) 90 90	16, 28, 46, 63	0
1	N	232/286 (81%)	-0.36	3 (1%) 74 73	20, 33, 51, 76	0
1	O	228/286 (79%)	-0.53	1 (0%) 90 90	19, 30, 47, 68	0
1	P	230/286 (80%)	-0.47	4 (1%) 67 65	18, 31, 53, 68	0
All	All	3659/4576 (79%)	-0.43	35 (0%) 79 79	16, 32, 54, 76	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	CYS	4.6
1	G	70	CYS	4.5
1	H	70	CYS	4.0
1	I	71	HIS	3.8
1	M	3	PRO	3.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	EDO	E	283	4/4	0.45	22.61	55,55,55,59	0
6	EDO	P	283	4/4	0.44	20.70	43,44,45,48	0
5	5AD	G	283	18/18	0.44	7.01	55,68,72,72	0
4	DHL	O	601	4/4	0.25	5.74	29,30,32,35	4
4	DHL	G	601	4/4	0.33	5.67	57,59,61,64	0
4	DHL	I	601	4/4	0.36	5.65	41,42,42,42	4
5	5AD	I	283	18/18	0.40	5.37	59,64,71,73	0
4	DHL	D	601	4/4	0.34	4.48	62,62,63,64	0
4	DHL	M	601	4/4	0.26	4.11	54,55,56,56	0
4	DHL	N	601	4/4	0.21	3.89	51,55,58,61	0
4	DHL	J	601	4/4	0.23	2.94	43,47,51,54	0
4	DHL	K	601	4/4	0.18	2.90	50,51,51,53	0
5	5AD	M	401	18/18	0.16	2.77	26,34,40,43	0
5	5AD	B	401	18/18	0.18	2.55	35,40,43,43	0
6	EDO	P	284	4/4	0.32	2.46	48,49,49,53	0
3	FLC	B	501	13/13	0.18	2.35	53,54,55,55	0
4	DHL	A	601	4/4	0.29	2.21	79,79,79,80	0
5	5AD	H	401	18/18	0.17	2.18	23,29,38,38	0
5	5AD	D	401	18/18	0.20	2.13	31,35,47,48	0
4	DHL	F	601	4/4	0.27	1.84	52,52,53,54	0
4	DHL	P	601	4/4	0.14	1.82	38,38,38,40	0
5	5AD	L	401	18/18	0.18	1.80	24,32,44,47	0
4	DHL	C	601	4/4	0.22	1.78	22,23,25,30	4
5	5AD	O	401	18/18	0.17	1.73	25,31,35,39	0
5	5AD	N	401	18/18	0.16	1.52	22,31,39,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	5AD	K	401	18/18	0.16	1.44	23,32,34,35	0
3	FLC	D	501	13/13	0.14	1.36	43,44,45,45	0
5	5AD	J	401	18/18	0.18	1.35	22,28,37,38	0
5	5AD	G	401	18/18	0.15	1.32	28,32,38,39	0
4	DHL	L	601	4/4	0.16	1.20	51,51,51,51	0
5	5AD	I	401	18/18	0.14	1.17	28,34,38,39	0
3	FLC	C	501	13/13	0.16	1.16	61,62,63,63	0
5	5AD	F	401	18/18	0.16	1.13	24,31,35,38	0
3	FLC	E	501	13/13	0.13	1.07	36,37,38,38	0
5	5AD	E	401	18/18	0.15	1.03	24,31,38,38	0
5	5AD	A	401	18/18	0.17	1.00	41,44,47,49	0
4	DHL	H	601	4/4	0.12	0.94	39,40,41,42	0
5	5AD	C	401	18/18	0.16	0.92	31,39,46,46	0
3	FLC	H	501	13/13	0.13	0.82	37,38,39,39	0
5	5AD	P	401	18/18	0.14	0.82	26,32,36,37	0
3	FLC	L	501	13/13	0.12	0.72	35,35,36,37	0
3	FLC	K	501	13/13	0.13	0.67	37,38,39,39	0
3	FLC	N	501	13/13	0.13	0.51	38,39,40,41	0
3	FLC	P	501	13/13	0.14	0.50	39,40,41,42	0
3	FLC	O	501	13/13	0.13	0.39	36,37,38,38	0
3	FLC	G	501	13/13	0.13	0.33	33,34,35,36	0
3	FLC	J	501	13/13	0.12	0.16	35,36,37,38	0
2	B12	N	301	91/91	0.11	0.06	15,23,29,32	0
2	B12	K	301	91/91	0.10	-0.11	17,25,29,34	0
2	B12	M	301	91/91	0.11	-0.14	10,21,28,31	0
2	B12	J	301	91/91	0.11	-0.16	18,23,30,32	0
3	FLC	I	501	13/13	0.11	-0.16	34,34,35,36	0
2	B12	D	301	91/91	0.12	-0.19	17,28,37,38	0
2	B12	P	301	91/91	0.11	-0.20	17,24,29,31	0
2	B12	L	301	91/91	0.11	-0.27	14,20,28,30	0
2	B12	G	301	91/91	0.11	-0.32	15,21,28,29	0
2	B12	E	301	91/91	0.10	-0.33	17,23,30,32	0
2	B12	H	301	91/91	0.10	-0.35	16,22,26,29	0
2	B12	O	301	91/91	0.10	-0.36	15,22,29,32	0
2	B12	I	301	91/91	0.11	-0.38	17,23,30,33	0
2	B12	A	301	91/91	0.12	-0.39	27,33,41,44	0
2	B12	B	301	91/91	0.12	-0.39	29,35,42,49	0
3	FLC	A	501	13/13	0.12	-0.40	43,44,45,46	0
2	B12	F	301	91/91	0.10	-0.43	12,21,28,30	0
3	FLC	F	501	13/13	0.10	-0.55	31,32,33,33	0
2	B12	C	301	91/91	0.12	-0.55	28,35,46,55	0
3	FLC	M	501	13/13	0.11	-0.80	35,36,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.