



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:37 AM BST

PDB ID : 4IT1
Title : Crystal structure of enolase pfl01_3283 (target efi-502286) from pseudomonas fluorescens pf0-1 with bound magnesium, potassium and tartrate
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Al Obaidi, N.; Stead, M.; Love, J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2013-01-17
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

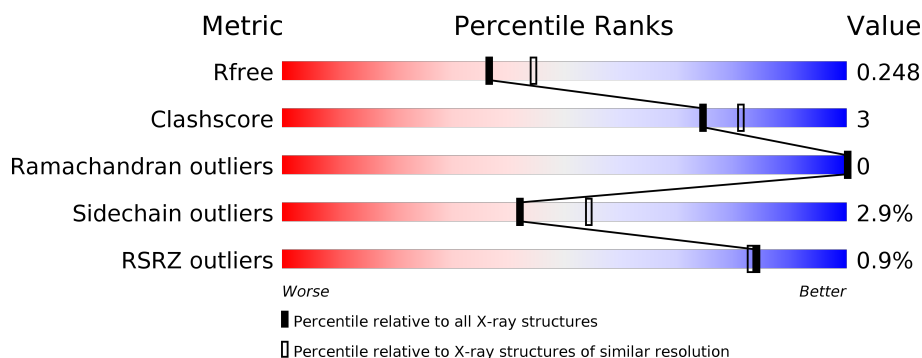
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	446	
1	B	446	
1	C	446	
1	D	446	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14027 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 Putative glucarate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3320	2109	574	622	15			
1	B	425	Total	C	N	O	S	0	4	0
			3325	2113	576	621	15			
1	C	426	Total	C	N	O	S	0	3	0
			3333	2118	580	620	15			
1	D	427	Total	C	N	O	S	0	7	0
			3364	2138	586	625	15			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP Q3KB33
A	-20	HIS	-	EXPRESSION TAG	UNP Q3KB33
A	-19	HIS	-	EXPRESSION TAG	UNP Q3KB33
A	-18	HIS	-	EXPRESSION TAG	UNP Q3KB33
A	-17	HIS	-	EXPRESSION TAG	UNP Q3KB33
A	-16	HIS	-	EXPRESSION TAG	UNP Q3KB33
A	-15	HIS	-	EXPRESSION TAG	UNP Q3KB33
A	-14	SER	-	EXPRESSION TAG	UNP Q3KB33
A	-13	SER	-	EXPRESSION TAG	UNP Q3KB33
A	-12	GLY	-	EXPRESSION TAG	UNP Q3KB33
A	-11	VAL	-	EXPRESSION TAG	UNP Q3KB33
A	-10	ASP	-	EXPRESSION TAG	UNP Q3KB33
A	-9	LEU	-	EXPRESSION TAG	UNP Q3KB33
A	-8	GLY	-	EXPRESSION TAG	UNP Q3KB33
A	-7	THR	-	EXPRESSION TAG	UNP Q3KB33
A	-6	GLU	-	EXPRESSION TAG	UNP Q3KB33
A	-5	ASN	-	EXPRESSION TAG	UNP Q3KB33
A	-4	LEU	-	EXPRESSION TAG	UNP Q3KB33
A	-3	TYR	-	EXPRESSION TAG	UNP Q3KB33
A	-2	PHE	-	EXPRESSION TAG	UNP Q3KB33
A	-1	GLN	-	EXPRESSION TAG	UNP Q3KB33

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q3KB33
B	-21	MET	-	EXPRESSION TAG	UNP Q3KB33
B	-20	HIS	-	EXPRESSION TAG	UNP Q3KB33
B	-19	HIS	-	EXPRESSION TAG	UNP Q3KB33
B	-18	HIS	-	EXPRESSION TAG	UNP Q3KB33
B	-17	HIS	-	EXPRESSION TAG	UNP Q3KB33
B	-16	HIS	-	EXPRESSION TAG	UNP Q3KB33
B	-15	HIS	-	EXPRESSION TAG	UNP Q3KB33
B	-14	SER	-	EXPRESSION TAG	UNP Q3KB33
B	-13	SER	-	EXPRESSION TAG	UNP Q3KB33
B	-12	GLY	-	EXPRESSION TAG	UNP Q3KB33
B	-11	VAL	-	EXPRESSION TAG	UNP Q3KB33
B	-10	ASP	-	EXPRESSION TAG	UNP Q3KB33
B	-9	LEU	-	EXPRESSION TAG	UNP Q3KB33
B	-8	GLY	-	EXPRESSION TAG	UNP Q3KB33
B	-7	THR	-	EXPRESSION TAG	UNP Q3KB33
B	-6	GLU	-	EXPRESSION TAG	UNP Q3KB33
B	-5	ASN	-	EXPRESSION TAG	UNP Q3KB33
B	-4	LEU	-	EXPRESSION TAG	UNP Q3KB33
B	-3	TYR	-	EXPRESSION TAG	UNP Q3KB33
B	-2	PHE	-	EXPRESSION TAG	UNP Q3KB33
B	-1	GLN	-	EXPRESSION TAG	UNP Q3KB33
B	0	SER	-	EXPRESSION TAG	UNP Q3KB33
C	-21	MET	-	EXPRESSION TAG	UNP Q3KB33
C	-20	HIS	-	EXPRESSION TAG	UNP Q3KB33
C	-19	HIS	-	EXPRESSION TAG	UNP Q3KB33
C	-18	HIS	-	EXPRESSION TAG	UNP Q3KB33
C	-17	HIS	-	EXPRESSION TAG	UNP Q3KB33
C	-16	HIS	-	EXPRESSION TAG	UNP Q3KB33
C	-15	HIS	-	EXPRESSION TAG	UNP Q3KB33
C	-14	SER	-	EXPRESSION TAG	UNP Q3KB33
C	-13	SER	-	EXPRESSION TAG	UNP Q3KB33
C	-12	GLY	-	EXPRESSION TAG	UNP Q3KB33
C	-11	VAL	-	EXPRESSION TAG	UNP Q3KB33
C	-10	ASP	-	EXPRESSION TAG	UNP Q3KB33
C	-9	LEU	-	EXPRESSION TAG	UNP Q3KB33
C	-8	GLY	-	EXPRESSION TAG	UNP Q3KB33
C	-7	THR	-	EXPRESSION TAG	UNP Q3KB33
C	-6	GLU	-	EXPRESSION TAG	UNP Q3KB33
C	-5	ASN	-	EXPRESSION TAG	UNP Q3KB33
C	-4	LEU	-	EXPRESSION TAG	UNP Q3KB33
C	-3	TYR	-	EXPRESSION TAG	UNP Q3KB33

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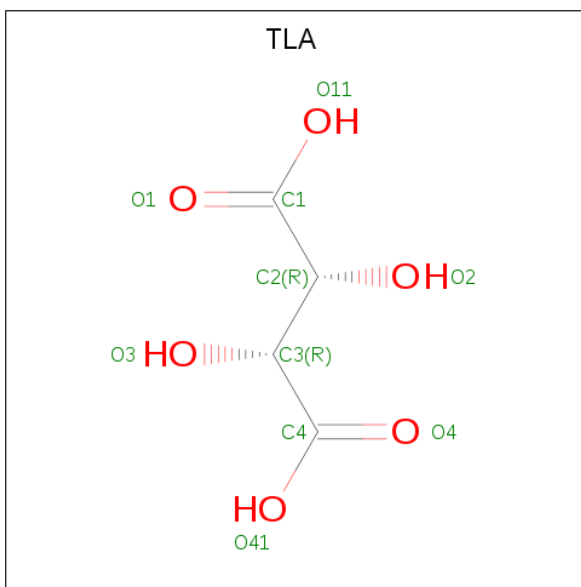
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	EXPRESSION TAG	UNP Q3KB33
C	-1	GLN	-	EXPRESSION TAG	UNP Q3KB33
C	0	SER	-	EXPRESSION TAG	UNP Q3KB33
D	-21	MET	-	EXPRESSION TAG	UNP Q3KB33
D	-20	HIS	-	EXPRESSION TAG	UNP Q3KB33
D	-19	HIS	-	EXPRESSION TAG	UNP Q3KB33
D	-18	HIS	-	EXPRESSION TAG	UNP Q3KB33
D	-17	HIS	-	EXPRESSION TAG	UNP Q3KB33
D	-16	HIS	-	EXPRESSION TAG	UNP Q3KB33
D	-15	HIS	-	EXPRESSION TAG	UNP Q3KB33
D	-14	SER	-	EXPRESSION TAG	UNP Q3KB33
D	-13	SER	-	EXPRESSION TAG	UNP Q3KB33
D	-12	GLY	-	EXPRESSION TAG	UNP Q3KB33
D	-11	VAL	-	EXPRESSION TAG	UNP Q3KB33
D	-10	ASP	-	EXPRESSION TAG	UNP Q3KB33
D	-9	LEU	-	EXPRESSION TAG	UNP Q3KB33
D	-8	GLY	-	EXPRESSION TAG	UNP Q3KB33
D	-7	THR	-	EXPRESSION TAG	UNP Q3KB33
D	-6	GLU	-	EXPRESSION TAG	UNP Q3KB33
D	-5	ASN	-	EXPRESSION TAG	UNP Q3KB33
D	-4	LEU	-	EXPRESSION TAG	UNP Q3KB33
D	-3	TYR	-	EXPRESSION TAG	UNP Q3KB33
D	-2	PHE	-	EXPRESSION TAG	UNP Q3KB33
D	-1	GLN	-	EXPRESSION TAG	UNP Q3KB33
D	0	SER	-	EXPRESSION TAG	UNP Q3KB33

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).

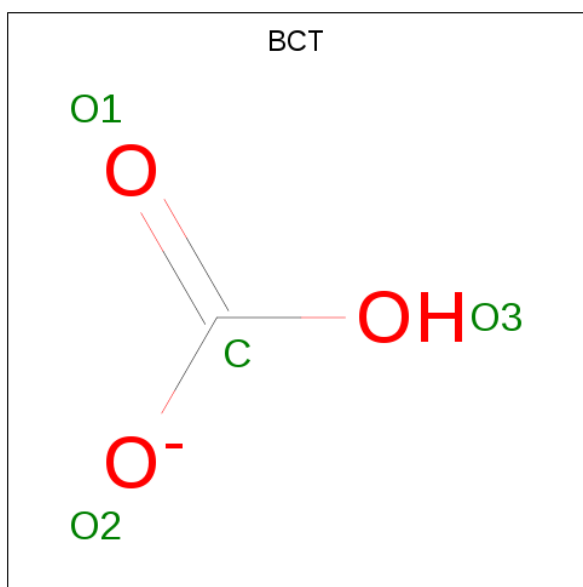


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	1	3		

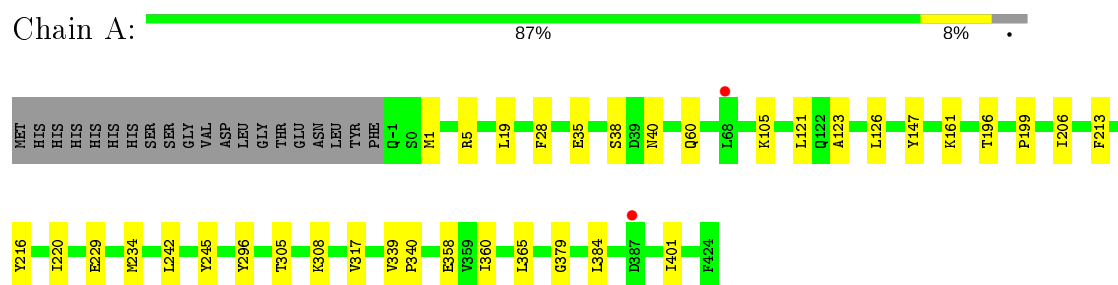
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total	O	0	1
			99	99		
6	B	93	Total	O	0	0
			93	93		
6	C	160	Total	O	0	0
			160	160		
6	D	282	Total	O	0	3
			285	285		

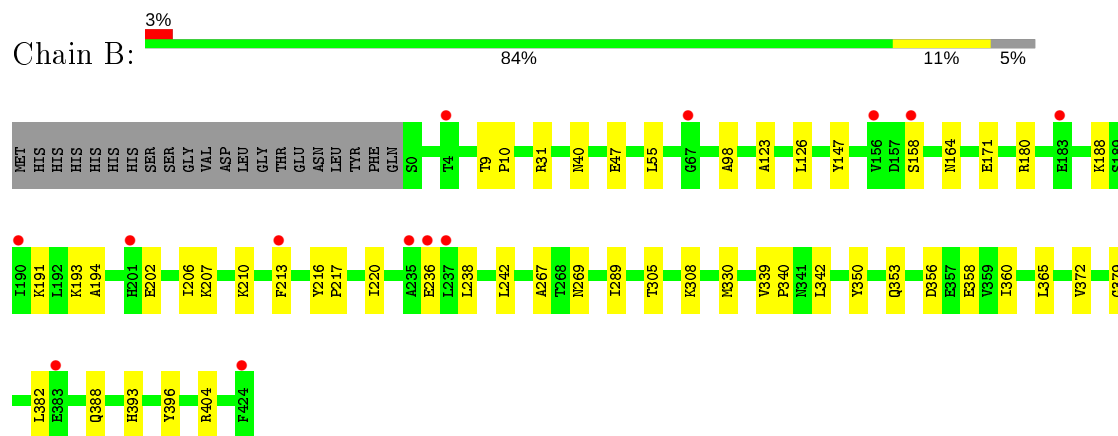
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

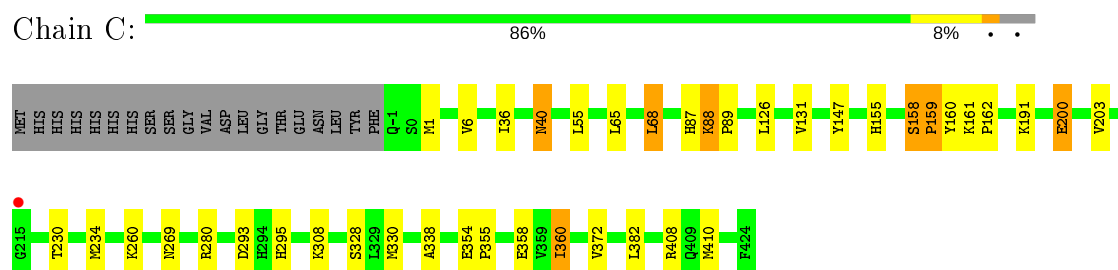
- Molecule 1: Putative glucarate dehydratase



- Molecule 1: Putative glucarate dehydratase



- Molecule 1: Putative glucarate dehydratase



- Molecule 1: Putative glucarate dehydratase

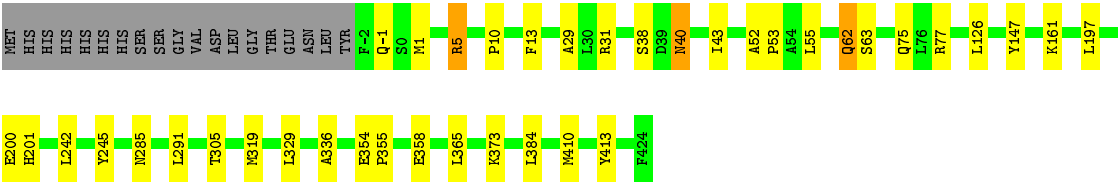
Chain D:

87%

8%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.32Å 147.69Å 173.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.40 – 2.20 47.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.40-2.20) 99.7 (47.36-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.194 , 0.250 0.194 , 0.248	Depositor DCC
R_{free} test set	3223 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14027	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BCT, MG, TLA, K

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	0.36	0/3406	0.54	0/4630
1	B	0.34	0/3417	0.51	0/4644
1	C	0.41	2/3422 (0.1%)	0.56	2/4649 (0.0%)
1	D	0.42	0/3465	0.58	0/4705
All	All	0.38	2/13710 (0.0%)	0.55	2/18628 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	PRO	N-CD	5.36	1.55	1.47
1	C	89	PRO	N-CD	5.00	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	LYS	C-N-CD	5.84	140.68	128.40
1	C	158	SER	C-N-CD	5.58	140.12	128.40

There are no chirality outliers.

There are no planarity outliers.

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	3320	0	3271	18	0
1	B	3325	0	3288	30	0
1	C	3333	0	3301	23	0
1	D	3364	0	3340	22	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	D	4	0	0	0	0
6	A	99	0	0	1	0
6	B	93	0	0	1	0
6	C	160	0	0	2	0
6	D	285	0	0	3	0
All	All	14027	0	13216	85	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 3.

All (85) 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:B:358:GLU:O	1:B:388:GLN:HG2	1.74	0.87
1:A:126:LEU:HD11	1:B:126:LEU:HD11	1.61	0.82
1:C:155:HIS:O	1:C:158:SER:HB2	1.87	0.75
1:A:19:LEU:HB3	1:A:196:THR:HG21	1.72	0.70
1:A:206:ILE:HD11	1:A:220:ILE:HG21	1.77	0.66
1:B:191:LYS:HD2	6:B:688:HOH:O	1.97	0.64
1:C:191:LYS:NZ	6:C:680:HOH:O	2.31	0.63
1:B:353[B]:GLN:HA	1:B:353[B]:GLN:NE2	2.16	0.61
1:B:330:MET:HE1	1:B:372:VAL:HG11	1.81	0.61
1:C:200:GLU:HA	1:C:234:MET:HE1	1.82	0.60
1:B:123:ALA:HB3	1:B:379:GLY:HA2	1.83	0.59
1:C:360:ILE:HD13	1:C:382:LEU:HD22	1.84	0.59
1:B:213:PHE:HB3	1:B:216:TYR:CD1	2.38	0.59
1:C:126:LEU:HD21	1:D:126:LEU:HG	1.85	0.59
1:C:358:GLU:HG3	1:C:360:ILE:HG13	1.85	0.58
1:D:10:PRO:HB3	1:D:55:LEU:HD11	1.84	0.58
1:C:126:LEU:HD11	1:D:126:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ASP:O	1:B:388:GLN:NE2	2.37	0.57
1:C:330:MET:HE1	1:C:372:VAL:HG11	1.86	0.56
1:C:230:THR:O	1:C:234:MET:HG2	2.05	0.56
1:D:31:ARG:NH1	6:D:852:HOH:O	2.37	0.56
1:A:213:PHE:HB3	1:A:216:TYR:CD1	2.41	0.55
1:D:52:ALA:HB3	1:D:53:PRO:HD3	1.89	0.54
1:B:10:PRO:HB3	1:B:55:LEU:HD11	1.90	0.54
1:D:329:LEU:HD23	1:D:365:LEU:HD11	1.91	0.52
1:C:308:LYS:HG2	1:D:305:THR:HG21	1.91	0.52
1:B:330:MET:HE2	1:B:365:LEU:HD13	1.91	0.52
1:C:126:LEU:HG	1:D:126:LEU:HD21	1.91	0.52
1:B:206:ILE:CD1	1:B:220:ILE:HB	2.39	0.51
1:D:410:MET:HE3	1:D:413:TYR:HB2	1.92	0.51
1:B:123:ALA:CB	1:B:379:GLY:HA2	2.41	0.50
1:B:98:ALA:HB2	1:B:404:ARG:HD3	1.93	0.50
1:D:1:MET:HE2	1:D:38:SER:CB	2.41	0.50
1:D:319:MET:HG3	1:D:336:ALA:HB2	1.92	0.50
1:B:164:ASN:HB2	1:B:180:ARG:HH12	1.76	0.49
1:C:159:PRO:HG2	1:C:160:TYR:CD2	2.48	0.49
1:A:308:LYS:HG2	1:B:305:THR:HG21	1.94	0.49
1:A:126:LEU:HG	1:B:126:LEU:HD21	1.94	0.48
1:A:199:PRO:HB2	1:A:234:MET:SD	2.53	0.48
1:D:77[B]:ARG:NH2	6:D:734:HOH:O	2.45	0.48
1:A:229:GLU:HG2	6:A:667:HOH:O	2.13	0.48
1:A:305:THR:HG21	1:B:308:LYS:HG2	1.95	0.48
1:A:123:ALA:CB	1:A:379:GLY:HA2	2.44	0.48
1:B:339:VAL:CG2	1:B:342:LEU:HB2	2.44	0.48
1:D:38:SER:OG	1:D:40:ASN:ND2	2.47	0.48
1:B:353[B]:GLN:HA	1:B:353[B]:GLN:HE21	1.79	0.47
1:C:203:VAL:HG21	1:C:234:MET:HE3	1.95	0.47
1:C:293:ASP:OD1	1:C:295:HIS:HD2	1.98	0.47
1:D:40:ASN:N	1:D:40:ASN:HD22	2.12	0.47
1:B:360:ILE:HD13	1:B:382:LEU:HD22	1.97	0.46
1:D:410:MET:CE	1:D:413:TYR:HB2	2.45	0.46
1:A:28:PHE:HB2	1:A:401:ILE:HD12	1.98	0.46
1:B:188:LYS:O	1:B:217:PRO:HD2	2.16	0.46
1:A:339:VAL:HA	1:A:340:PRO:HD3	1.83	0.46
1:B:31:ARG:HE	1:B:47:GLU:HG2	1.80	0.46
1:C:65:LEU:O	1:C:68:LEU:HB2	2.16	0.46
1:A:105:LYS:HD2	1:A:296:TYR:HB2	1.99	0.45
1:B:207:LYS:O	1:B:210:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:HG23	1:C:338:ALA:HB2	1.99	0.45
1:A:1:MET:HE2	1:A:38:SER:CB	2.46	0.44
1:C:295:HIS:HE1	1:C:328:SER:OG	2.01	0.44
1:D:354:GLU:HA	1:D:355:PRO:HD3	1.91	0.44
1:C:6:VAL:HG13	1:C:36:ILE:HD13	1.99	0.43
1:C:40:ASN:HD22	1:C:40:ASN:H	1.65	0.43
1:C:161:LYS:HA	1:C:162:PRO:HD2	1.85	0.43
1:D:197:LEU:HD23	1:D:201:HIS:HD2	1.83	0.43
1:D:5:ARG:NH2	6:D:817:HOH:O	2.52	0.43
1:B:238:LEU:HD13	1:B:242:LEU:HD11	2.01	0.42
1:A:242:LEU:HD12	1:A:245:TYR:CZ	2.54	0.42
1:D:40:ASN:H	1:D:40:ASN:HD22	1.66	0.42
1:B:9:THR:HA	1:B:10:PRO:HD2	1.96	0.42
1:B:194:ALA:HB1	1:B:202:GLU:OE1	2.20	0.42
1:B:393:HIS:O	1:B:396:TYR:HB3	2.20	0.42
1:A:35:GLU:HG3	1:A:384:LEU:HD12	2.02	0.41
1:B:206:ILE:HD12	1:B:220:ILE:HD12	2.02	0.41
1:A:358:GLU:OE2	1:A:360:ILE:HG12	2.20	0.41
1:A:123:ALA:HB3	1:A:379:GLY:HA2	2.03	0.41
1:C:280:ARG:HD2	6:C:648:HOH:O	2.20	0.41
1:C:354:GLU:HA	1:C:355:PRO:HD3	1.95	0.41
1:B:339:VAL:HA	1:B:340:PRO:HD3	1.93	0.41
1:D:62:GLN:HG2	1:D:63:SER:N	2.36	0.41
1:B:267:ALA:HA	1:B:289:ILE:O	2.21	0.41
1:D:13:PHE:CE1	1:D:29:ALA:HB3	2.56	0.41
1:C:87:HIS:HD2	1:C:88:LYS:O	2.04	0.40
1:D:242:LEU:HD12	1:D:245:TYR:CZ	2.57	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	426/446 (96%)	406 (95%)	20 (5%)	0	100	100
1	B	427/446 (96%)	420 (98%)	7 (2%)	0	100	100
1	C	427/446 (96%)	418 (98%)	9 (2%)	0	100	100
1	D	432/446 (97%)	423 (98%)	9 (2%)	0	100	100
All	All	1712/1784 (96%)	1667 (97%)	45 (3%)	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	351/369 (95%)	343 (98%)	8 (2%)	50	63
1	B	353/369 (96%)	345 (98%)	8 (2%)	50	63
1	C	353/369 (96%)	342 (97%)	11 (3%)	40	51
1	D	357/369 (97%)	343 (96%)	14 (4%)	32	41
All	All	1414/1476 (96%)	1373 (97%)	41 (3%)	42	54

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	40	ASN
1	A	60	GLN
1	A	121	LEU
1	A	147	TYR
1	A	161	LYS
1	A	317	VAL
1	A	365	LEU
1	B	40	ASN
1	B	147	TYR
1	B	158	SER
1	B	171	GLU
1	B	193	LYS

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Mol	Chain	Res	Type
1	B	236	GLU
1	B	269	ASN
1	B	350	TYR
1	C	1	MET
1	C	40	ASN
1	C	55	LEU
1	C	68	LEU
1	C	147	TYR
1	C	200	GLU
1	C	260	LYS
1	C	269	ASN
1	C	360	ILE
1	C	408	ARG
1	C	410	MET
1	D	-1	GLN
1	D	5	ARG
1	D	40	ASN
1	D	43	ILE
1	D	62	GLN
1	D	75	GLN
1	D	147	TYR
1	D	161	LYS
1	D	200	GLU
1	D	285	ASN
1	D	291	LEU
1	D	358	GLU
1	D	373	LYS
1	D	384	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	81	GLN
1	A	102	HIS
1	A	127	ASN
1	A	284	GLN
1	A	304	GLN
1	B	40	ASN
1	B	58	GLN
1	B	59	GLN
1	B	81	GLN

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Mol	Chain	Res	Type
1	B	154	GLN
1	B	201	HIS
1	B	284	GLN
1	B	294	HIS
1	C	40	ASN
1	C	59	GLN
1	C	81	GLN
1	C	87	HIS
1	C	284	GLN
1	C	295	HIS
1	D	40	ASN
1	D	59	GLN
1	D	60	GLN
1	D	81	GLN
1	D	304	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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
3	TLA	C	501	-	3,9,9	1.00	0	6,12,12	2.03	3 (50%)
5	BCT	D	503	-	0,3,3	0.00	-	0,3,3	0.00	-
3	TLA	D	502	-	3,9,9	0.81	0	6,12,12	1.66	2 (33%)
3	TLA	A	502	-	3,9,9	0.79	0	6,12,12	1.59	2 (33%)
3	TLA	B	501	-	3,9,9	0.41	0	6,12,12	0.89	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
3	TLA	C	501	-	-	0/4/12/12	-
3	TLA	D	502	-	-	1/4/12/12	-
3	TLA	A	502	-	-	0/4/12/12	-
3	TLA	B	501	-	-	0/4/12/12	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	TLA	C1-C2-C3	-3.02	106.61	113.11
3	C	501	TLA	O3-C3-C4	-2.99	103.91	111.10
3	D	502	TLA	O2-C2-C1	-2.64	104.75	111.10
3	C	501	TLA	C4-C3-C2	-2.51	107.71	113.11
3	D	502	TLA	O3-C3-C4	-2.43	105.26	111.10
3	A	502	TLA	C1-C2-C3	-2.34	108.07	113.11
3	A	502	TLA	C4-C3-C2	-2.25	108.27	113.11

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	TLA	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	426/446 (95%)	0.05	2 (0%) 91 90	36, 61, 87, 121	0
1	B	425/446 (95%)	0.22	13 (3%) 49 47	41, 65, 92, 112	0
1	C	426/446 (95%)	-0.28	1 (0%) 95 94	32, 49, 73, 105	0
1	D	427/446 (95%)	-0.28	0 100 100	24, 36, 55, 109	0
All	All	1704/1784 (95%)	-0.07	16 (0%) 84 83	24, 53, 86, 121	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	GLY	2.9
1	B	190	ILE	2.8
1	B	236	GLU	2.7
1	A	387	ASP	2.7
1	B	4	THR	2.7
1	B	158	SER	2.6
1	B	213	PHE	2.5
1	B	201	HIS	2.5
1	B	156	VAL	2.4
1	A	68	LEU	2.3
1	B	183	GLU	2.2
1	B	235	ALA	2.2
1	B	237	LEU	2.1
1	B	67	GLY	2.1
1	B	383	GLU	2.0
1	B	424	PHE	2.0

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 [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(\AA^2)	Q<0.9
5	BCT	D	503	4/4	0.87	0.31	57,66,67,77	0
2	MG	A	501	1/1	0.87	0.14	53,53,53,53	0
2	MG	D	501	1/1	0.91	0.14	35,35,35,35	0
4	K	B	502	1/1	0.92	0.05	66,66,66,66	0
3	TLA	B	501	10/10	0.94	0.14	55,61,73,91	0
3	TLA	A	502	10/10	0.95	0.09	50,66,77,80	0
3	TLA	D	502	10/10	0.96	0.08	34,42,48,53	0
3	TLA	C	501	10/10	0.97	0.08	44,52,68,71	0
4	K	C	502	1/1	0.99	0.07	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.