



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:15 AM UTC

PDB ID : 4IT1 / pdb_00004it1
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

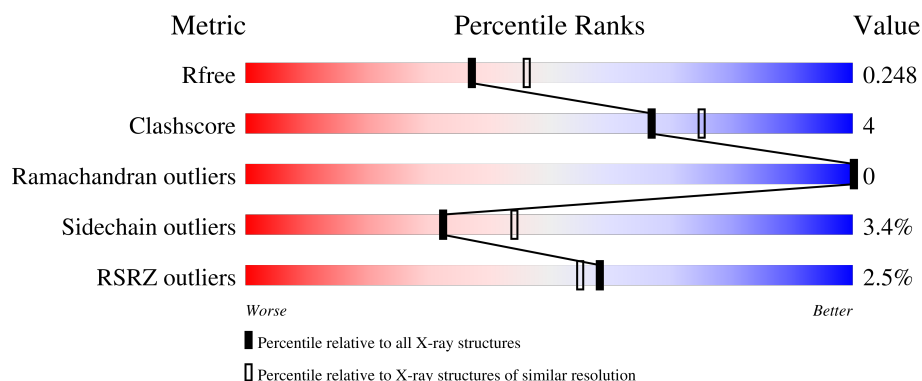
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 86% 9% .
1	B	446	3% 83% 11% . 5%
1	C	446	% 86% 8% . .
1	D	446	% 87% 8% . .

Validation Pipeline (wwPDB-VP) : 2.49

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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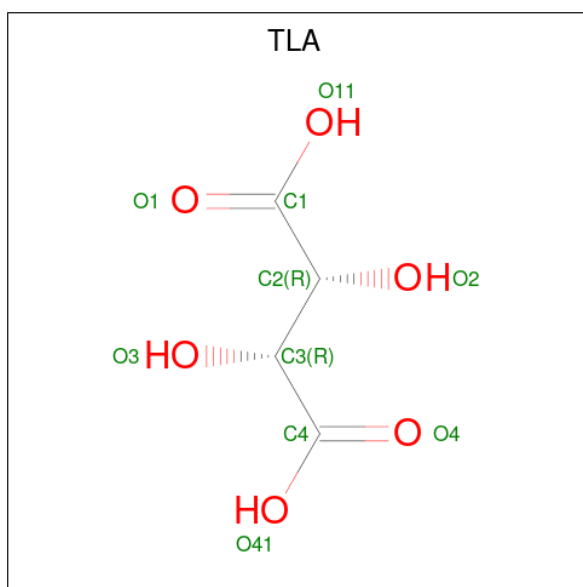
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP Q3KB33
C	-1	GLN	-	expression tag	UNP Q3KB33
C	0	SER	-	expression tag	UNP Q3KB33
D	-21	MET	-	expression tag	UNP Q3KB33
D	-20	HIS	-	expression tag	UNP Q3KB33
D	-19	HIS	-	expression 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 (CCD ID: 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 (CCD ID: TLA) (formula: C₄H₆O₆).

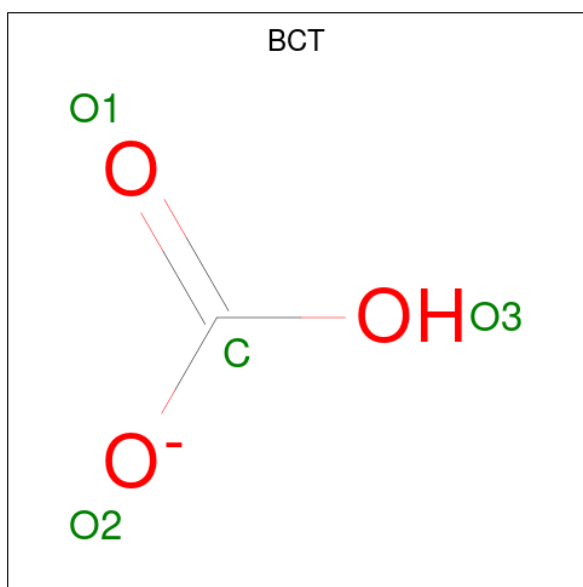


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is POTASSIUM ION (CCD ID: 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 (CCD ID: BCT) (formula: CHO_3).



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

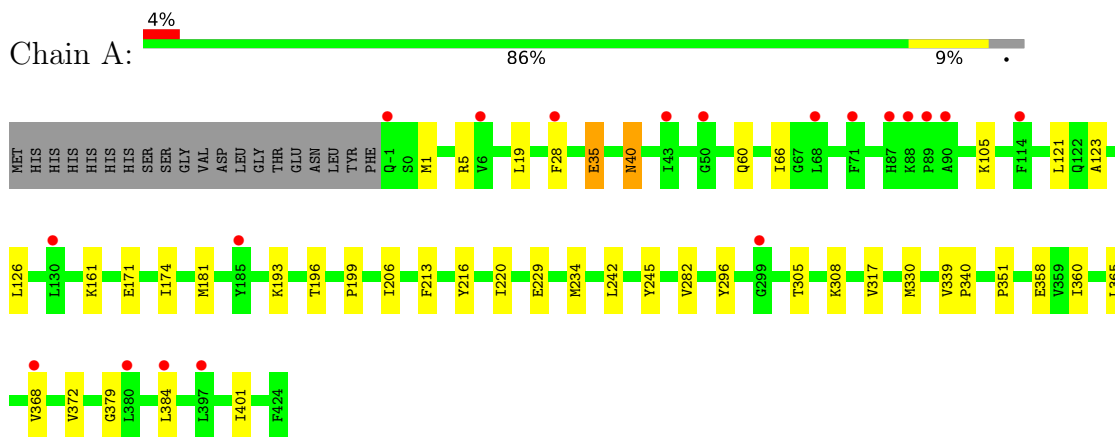
- Molecule 6 is water.

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		

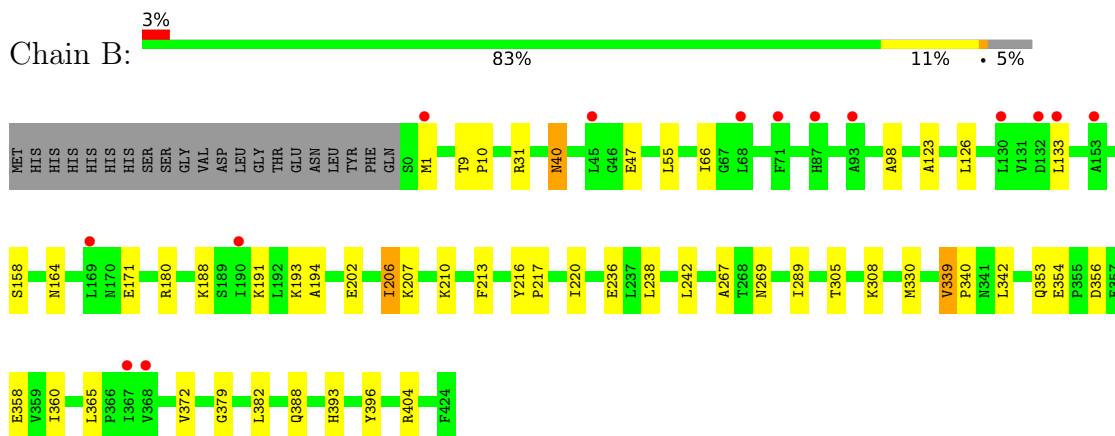
3 Residue-property plots

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.

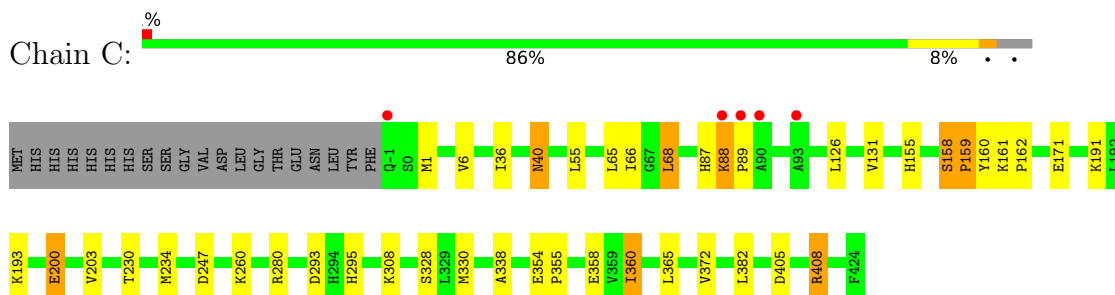
- Molecule 1: Putative glucarate dehydratase



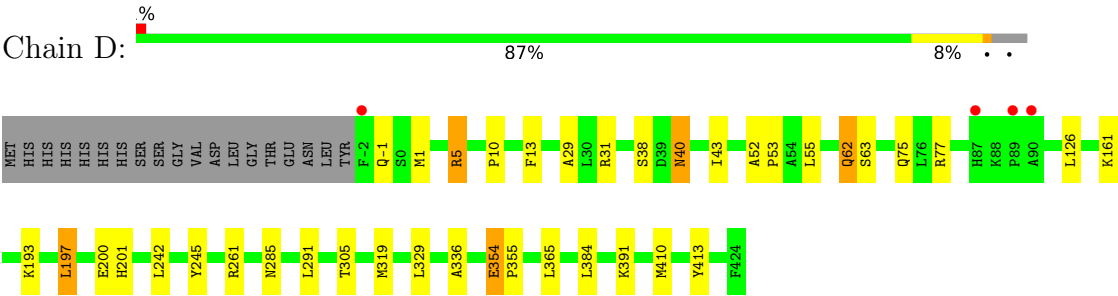
- Molecule 1: Putative glucarate dehydratase



- Molecule 1: Putative glucarate dehydratase



● Molecule 1: Putative glucarate dehydratase



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 47.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.40-2.20) 99.7 (47.40-2.20)	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 , 30.6	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: TLA, MG, BCT, 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	0.48	0/3406	0.84	0/4630
1	B	0.45	0/3417	0.82	2/4644 (0.0%)
1	C	0.56	5/3422 (0.1%)	0.83	4/4649 (0.1%)
1	D	0.56	0/3465	0.78	2/4705 (0.0%)
All	All	0.52	5/13710 (0.0%)	0.82	8/18628 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	SER	C-N	8.26	1.40	1.33
1	C	247	ASP	C-O	-7.95	1.20	1.23
1	C	88	LYS	C-N	6.29	1.41	1.33
1	C	159	PRO	N-CD	5.43	1.55	1.47
1	C	89	PRO	N-CD	5.08	1.54	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	SER	CA-C-N	-6.85	113.06	121.00
1	C	158	SER	C-N-CA	-6.85	113.06	121.00
1	C	88	LYS	CA-C-N	-6.68	112.62	119.83
1	C	88	LYS	C-N-CA	-6.68	112.62	119.83
1	D	354	GLU	CA-C-N	5.31	125.63	119.47
1	D	354	GLU	C-N-CA	5.31	125.63	119.47
1	B	354	GLU	CA-C-N	5.16	124.78	119.05
1	B	354	GLU	C-N-CA	5.16	124.78	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3320	0	3271	22	0
1	B	3325	0	3288	33	0
1	C	3333	0	3301	28	0
1	D	3364	0	3340	23	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	4	0
All	All	14027	0	13216	98	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 4.

All (98) 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:1:MET:HE3	1:A:40:ASN:HD21	1.50	0.74
1:C:203:VAL:HG21	1:C:234:MET:HE3	1.70	0.72
1:A:19:LEU:HB3	1:A:196:THR:HG21	1.72	0.70
1:D:1:MET:HE3	1:D:40:ASN:HD21	1.55	0.70
1:A:206:ILE:HD11	1:A:220:ILE:HG21	1.77	0.66
1:B:330:MET:HE3	1:B:365:LEU:HD13	1.78	0.66
1:C:330:MET:HE1	1:C:372:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:MET:HE1	1:C:372:VAL:CG1	2.27	0.65
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:330:MET:HE1	1:B:372:VAL:CG1	2.29	0.62
1:B:353[B]:GLN:NE2	1:B:353[B]:GLN:HA	2.16	0.61
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
1:C:330:MET:HE3	1:C:365:LEU:HD13	1.85	0.57
1:B:356:ASP:O	1:B:388:GLN:NE2	2.37	0.57
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:B:1:MET:HE3	1:B:40:ASN:HD21	1.71	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:410:MET:HE3	1:D:413:TYR:HB2	1.89	0.53
1:B:330:MET:HE1	1:B:372:VAL:HG11	1.90	0.53
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: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:A:330:MET:HE1	1:A:372:VAL:HG13	1.92	0.51
1:C:200:GLU:HA	1:C:234:MET:HE1	1.92	0.51
1:B:98:ALA:HB2	1:B:404:ARG:HD3	1.93	0.50
1:B:123:ALA:CB	1:B:379:GLY:HA2	2.41	0.50
1:A:181:MET:HE2	1:A:351:PRO:HB2	1.94	0.50
1:B:330:MET:HE1	1:B:372:VAL:HG13	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:293:ASP:OD1	1:C:295:HIS:HD2	1.98	0.47
1:D:40:ASN:HD22	1:D:40:ASN:N	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:C:203:VAL:CG2	1:C:234:MET:HE3	2.44	0.45
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
1:C:131:VAL:HG23	1:C:338:ALA:HB2	1.99	0.45
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:171:GLU:H	1:A:171:GLU:CD	2.26	0.42
1:A:242:LEU:HD12	1:A:245:TYR:CZ	2.54	0.42
1:D:40:ASN:HD22	1:D:40:ASN:H	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:330:MET:HE1	1:A:372:VAL:CG1	2.51	0.41
1:A:358:GLU:OE2	1:A:360:ILE:HG12	2.20	0.41
1:C:405:ASP:CG	1:C:408:ARG:HB3	2.45	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:267:ALA:HA	1:B:289:ILE:O	2.21	0.41
1:B:339:VAL:HA	1:B:340:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:MET:HE1	1:C:372:VAL:HG13	2.01	0.41
1:D:62:GLN:HG2	1:D:63:SER:N	2.36	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:391:LYS:NZ	6:D:803:HOH:O	2.55	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 [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	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 [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	351/369 (95%)	338 (96%)	13 (4%)	30	41
1	B	353/369 (96%)	343 (97%)	10 (3%)	38	52
1	C	353/369 (96%)	342 (97%)	11 (3%)	35	48
1	D	357/369 (97%)	343 (96%)	14 (4%)	28	39
All	All	1414/1476 (96%)	1366 (97%)	48 (3%)	32	44

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	35	GLU
1	A	40	ASN
1	A	60	GLN
1	A	66	ILE
1	A	121	LEU
1	A	161	LYS
1	A	174	ILE
1	A	193	LYS
1	A	282	VAL
1	A	317	VAL
1	A	365	LEU
1	A	368	VAL
1	B	40	ASN
1	B	66	ILE
1	B	133	LEU
1	B	158	SER
1	B	171	GLU
1	B	193	LYS
1	B	206	ILE
1	B	236	GLU
1	B	269	ASN
1	B	339	VAL
1	C	1	MET
1	C	40	ASN
1	C	55	LEU
1	C	66	ILE
1	C	68	LEU
1	C	171	GLU
1	C	193	LYS
1	C	200	GLU
1	C	260	LYS
1	C	360	ILE

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Mol	Chain	Res	Type
1	C	408	ARG
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	161	LYS
1	D	193	LYS
1	D	197	LEU
1	D	200	GLU
1	D	261	ARG
1	D	285	ASN
1	D	291	LEU
1	D	384	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	81	GLN
1	A	102	HIS
1	A	122	GLN
1	A	127	ASN
1	A	201	HIS
1	A	284	GLN
1	A	304	GLN
1	A	349	HIS
1	A	353	GLN
1	A	386	HIS
1	B	40	ASN
1	B	59	GLN
1	B	81	GLN
1	B	122	GLN
1	B	154	GLN
1	B	201	HIS
1	B	284	GLN
1	B	294	HIS
1	B	386	HIS
1	C	40	ASN
1	C	59	GLN
1	C	62	GLN

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Mol	Chain	Res	Type
1	C	64	GLN
1	C	81	GLN
1	C	87	HIS
1	C	284	GLN
1	C	295	HIS
1	C	304	GLN
1	C	388	GLN
1	D	40	ASN
1	D	59	GLN
1	D	62	GLN
1	D	81	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 oligosaccharides 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	$\# Z > 2$
5	BCT	D	503	-	3,3,3	0.52	0	2,3,3	0.79	0
3	TLA	C	501	-	9,9,9	2.26	4 (44%)	12,12,12	1.43	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TLA	A	502	-	9,9,9	1.77	4 (44%)	12,12,12	1.30	1 (8%)
3	TLA	D	502	-	9,9,9	2.04	4 (44%)	12,12,12	1.38	2 (16%)
3	TLA	B	501	-	9,9,9	1.21	0	12,12,12	0.97	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	D	502	-	-	0/12/12/12	-
3	TLA	C	501	-	-	2/12/12/12	-
3	TLA	A	502	-	-	2/12/12/12	-
3	TLA	B	501	-	-	1/12/12/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	TLA	C3-C4	-3.97	1.47	1.52
3	C	501	TLA	C2-C1	-3.54	1.47	1.52
3	D	502	TLA	C2-C1	-3.25	1.48	1.52
3	D	502	TLA	C3-C4	-3.16	1.48	1.52
3	D	502	TLA	O41-C4	-3.08	1.20	1.30
3	A	502	TLA	C2-C1	-2.86	1.48	1.52
3	C	501	TLA	O11-C1	-2.80	1.21	1.30
3	A	502	TLA	C3-C4	-2.69	1.48	1.52
3	C	501	TLA	O41-C4	-2.68	1.22	1.30
3	A	502	TLA	O41-C4	-2.57	1.22	1.30
3	D	502	TLA	O11-C1	-2.49	1.22	1.30
3	A	502	TLA	O11-C1	-2.12	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	TLA	O3-C3-C4	-3.17	103.91	110.69
3	D	502	TLA	O2-C2-C1	-2.78	104.75	110.69
3	D	502	TLA	O3-C3-C4	-2.54	105.26	110.69
3	A	502	TLA	O11-C1-C2	2.15	119.28	113.31
3	C	501	TLA	O11-C1-C2	2.13	119.22	113.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	TLA	C2-C3-C4-O4
3	C	501	TLA	C2-C3-C4-O4
3	C	501	TLA	C2-C3-C4-O41
3	A	502	TLA	C2-C3-C4-O41
3	B	501	TLA	O11-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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, 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%)	0.62	19 (4%) 38 35	36, 61, 87, 121	2 (0%)
1	B	425/446 (95%)	0.54	14 (3%) 49 46	29, 65, 92, 112	4 (0%)
1	C	426/446 (95%)	-0.11	5 (1%) 76 74	27, 49, 73, 105	3 (0%)
1	D	427/446 (95%)	-0.50	4 (0%) 81 79	19, 36, 55, 109	7 (1%)
All	All	1704/1784 (95%)	0.14	42 (2%) 58 55	19, 53, 86, 121	16 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	ALA	4.4
1	D	-2	PHE	4.0
1	D	89	PRO	3.7
1	C	-1	GLN	3.3
1	A	90	ALA	3.2
1	A	89	PRO	3.2
1	A	71	PHE	3.1
1	A	-1	GLN	2.9
1	C	93	ALA	2.9
1	A	43	ILE	2.8
1	C	89	PRO	2.8
1	D	87	HIS	2.7
1	A	68	LEU	2.6
1	B	190	ILE	2.6
1	A	380	LEU	2.6
1	A	50	GLY	2.5
1	A	397	LEU	2.5
1	B	132	ASP	2.5
1	A	114	PHE	2.5
1	B	93	ALA	2.4
1	A	130	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	368	VAL	2.3
1	A	88	LYS	2.3
1	A	185	TYR	2.3
1	C	88	LYS	2.3
1	A	384	LEU	2.2
1	B	130	LEU	2.2
1	B	133	LEU	2.2
1	B	169	LEU	2.2
1	A	28	PHE	2.2
1	A	368	VAL	2.2
1	B	45	LEU	2.2
1	B	71	PHE	2.2
1	A	299	GLY	2.2
1	B	367	ILE	2.1
1	A	87	HIS	2.1
1	B	153	ALA	2.1
1	C	90	ALA	2.1
1	A	6	VAL	2.1
1	B	1	MET	2.0
1	B	87	HIS	2.0
1	B	68	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	BCT	D	503	4/4	0.86	0.13	57,66,67,77	0
3	TLA	A	502	10/10	0.89	0.10	50,66,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TLA	D	502	10/10	0.93	0.08	34,42,48,53	0
4	K	B	502	1/1	0.93	0.12	66,66,66,66	0
3	TLA	B	501	10/10	0.93	0.09	55,61,73,91	0
3	TLA	C	501	10/10	0.95	0.07	44,52,68,71	0
2	MG	A	501	1/1	0.98	0.04	53,53,53,53	0
4	K	C	502	1/1	0.98	0.05	48,48,48,48	0
2	MG	D	501	1/1	0.98	0.04	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.