



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:28 AM UTC

PDB ID : 4OEC / pdb_00004oec
Title : Crystal structure of glycerophosphodiester phosphodiesterase from *Thermococcus kodakarensis* KOD1
Authors : Atsuta, Y.; You, D.J.; Takano, K.; Koga, Y.; Kanaya, S.
Deposited on : 2014-01-13
Resolution : 1.90 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
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)
Validation Pipeline (wwPDB-VP) : 2.49

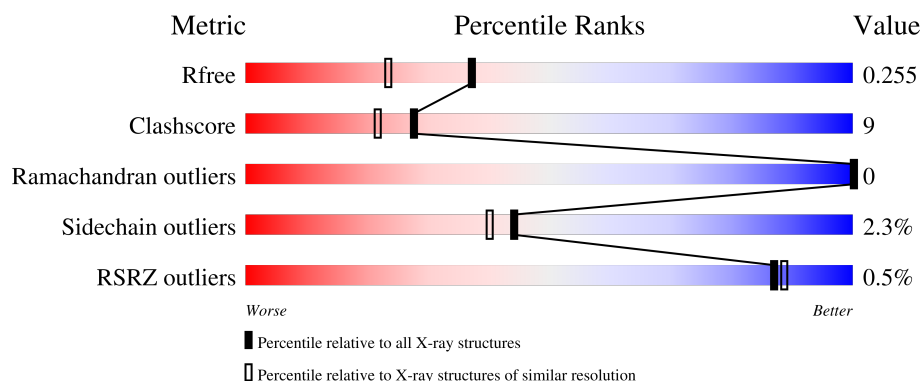
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	248	 68% 29% .
1	B	248	 71% 26% .
1	C	248	 2% 71% 25% .
1	D	248	 67% 29% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8713 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 Glycerophosphoryl diester phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			2004	1272	345	378	9			
1	B	248	Total	C	N	O	S	0	0	0
			2004	1272	345	378	9			
1	C	248	Total	C	N	O	S	0	0	0
			2004	1272	345	378	9			
1	D	248	Total	C	N	O	S	0	0	0
			2004	1272	345	378	9			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

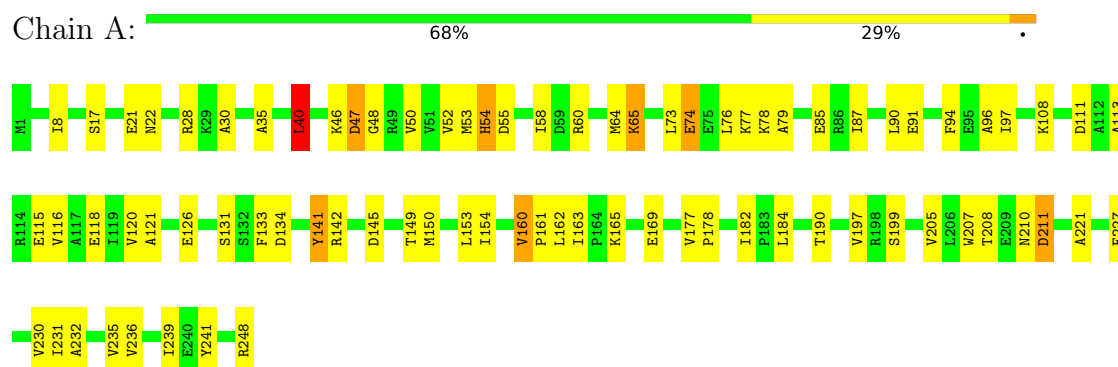
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total	O	0	0
			224	224		
3	B	185	Total	O	0	0
			185	185		
3	C	107	Total	O	0	0
			107	107		
3	D	177	Total	O	0	0
			177	177		

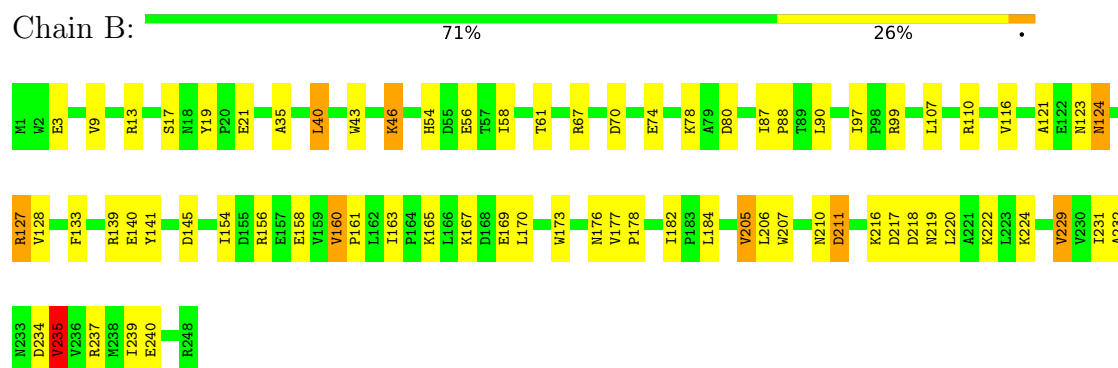
3 Residue-property plots

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.

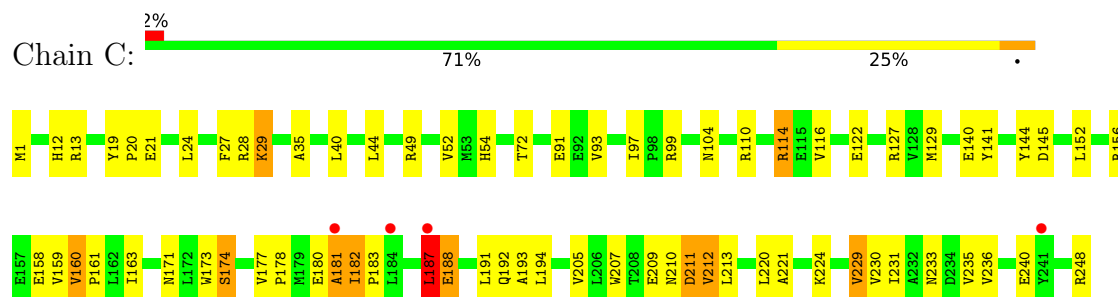
- Molecule 1: Glycerophosphoryl diester phosphodiesterase



- Molecule 1: Glycerophosphoryl diester phosphodiesterase



- Molecule 1: Glycerophosphoryl diester phosphodiesterase

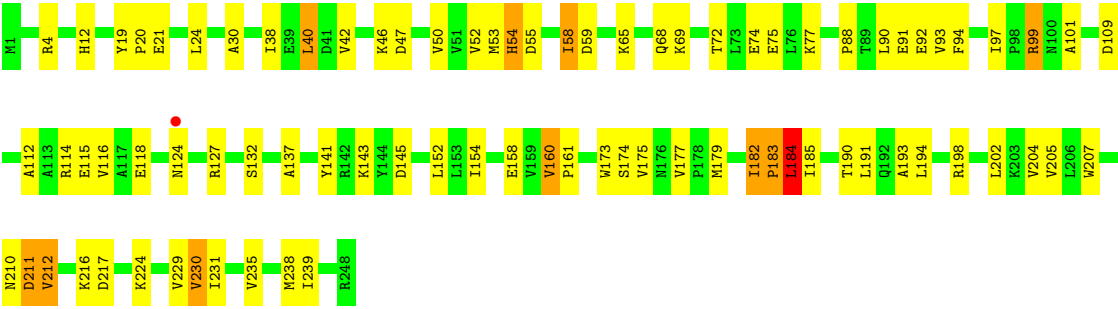


- Molecule 1: Glycerophosphoryl diester phosphodiesterase

Chain D:

67%

29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.72Å 132.03Å 171.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-1.90) 99.4 (50.00-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.250 0.200 , 0.255	Depositor DCC
R_{free} test set	4013 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.3	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	8713	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: MG

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	2.07	60/2035 (2.9%)	1.04	8/2750 (0.3%)
1	B	1.98	39/2035 (1.9%)	1.05	6/2750 (0.2%)
1	C	1.83	27/2035 (1.3%)	1.09	8/2750 (0.3%)
1	D	2.03	51/2035 (2.5%)	1.09	8/2750 (0.3%)
All	All	1.98	177/8140 (2.2%)	1.07	30/11000 (0.3%)

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	A	0	1
1	D	0	1
All	All	0	2

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	ILE	C-O	-10.77	1.15	1.24
1	C	21	GLU	C-N	-8.45	1.21	1.33
1	B	182	ILE	C-O	-8.33	1.17	1.24
1	D	91	GLU	C-N	-8.27	1.23	1.33
1	A	197	VAL	C-O	-7.98	1.14	1.24
1	A	120	VAL	C-O	-7.37	1.15	1.24
1	C	193	ALA	CA-CB	-7.17	1.42	1.53
1	B	177	VAL	C-O	-7.05	1.17	1.24
1	A	35	ALA	C-O	-6.92	1.15	1.23
1	A	30	ALA	CA-CB	-6.88	1.42	1.53
1	C	160	VAL	CA-CB	-6.87	1.49	1.53
1	A	47	ASP	C-N	-6.83	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	VAL	C-O	-6.82	1.17	1.24
1	C	27	PHE	C-O	-6.82	1.16	1.24
1	D	182	ILE	C-O	-6.79	1.18	1.24
1	C	97	ILE	C-O	-6.79	1.17	1.24
1	A	46	LYS	C-N	6.73	1.41	1.33
1	B	176	ASN	C-O	-6.72	1.16	1.24
1	B	46	LYS	C-O	-6.72	1.16	1.24
1	C	182	ILE	CA-CB	-6.70	1.50	1.54
1	D	231	ILE	C-O	-6.67	1.17	1.24
1	B	182	ILE	CA-CB	-6.66	1.50	1.54
1	A	177	VAL	C-O	-6.61	1.17	1.24
1	D	19	TYR	C-O	-6.59	1.18	1.24
1	A	141	TYR	C-O	-6.58	1.16	1.24
1	D	21	GLU	CB-CG	-6.56	1.32	1.52
1	D	46	LYS	C-O	-6.51	1.16	1.24
1	A	79	ALA	CA-CB	-6.42	1.43	1.53
1	A	230	VAL	C-O	-6.40	1.17	1.24
1	D	90	LEU	C-O	-6.40	1.16	1.24
1	D	207	TRP	C-O	-6.40	1.15	1.23
1	B	232	ALA	C-O	-6.39	1.16	1.23
1	B	19	TYR	C-O	-6.39	1.17	1.24
1	A	182	ILE	C-O	-6.33	1.19	1.24
1	A	221	ALA	C-O	-6.33	1.16	1.24
1	D	190	THR	C-O	-6.23	1.17	1.24
1	A	40	LEU	C-O	-6.14	1.16	1.23
1	D	224	LYS	C-O	-6.12	1.16	1.23
1	C	221	ALA	CA-CB	-6.09	1.43	1.53
1	B	154	ILE	C-O	-6.04	1.17	1.24
1	D	239	ILE	C-O	-6.02	1.17	1.24
1	A	205	VAL	C-O	-6.01	1.17	1.24
1	B	205	VAL	C-O	-6.00	1.17	1.24
1	B	43	TRP	C-O	-5.98	1.16	1.23
1	C	152	LEU	C-O	-5.97	1.16	1.24
1	D	205	VAL	C-O	-5.97	1.18	1.24
1	B	58	ILE	C-O	-5.95	1.17	1.24
1	A	131	SER	C-O	-5.95	1.16	1.23
1	D	52	VAL	C-O	-5.93	1.17	1.24
1	D	93	VAL	C-O	-5.92	1.17	1.24
1	B	13	ARG	C-O	-5.91	1.16	1.23
1	D	74	GLU	C-O	-5.90	1.17	1.24
1	A	46	LYS	C-O	-5.90	1.16	1.24
1	A	94	PHE	C-O	-5.87	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	VAL	C-O	-5.86	1.17	1.24
1	B	231	ILE	C-O	-5.86	1.17	1.24
1	D	229	VAL	C-O	-5.85	1.18	1.24
1	D	132	SER	C-O	-5.85	1.16	1.23
1	D	30	ALA	C-O	-5.84	1.17	1.24
1	A	50	VAL	C-O	-5.82	1.17	1.24
1	B	206	LEU	C-O	-5.81	1.16	1.24
1	D	112	ALA	C-O	-5.79	1.16	1.24
1	A	77	LYS	C-O	-5.79	1.16	1.24
1	D	118	GLU	C-O	-5.78	1.17	1.24
1	A	165	LYS	C-O	-5.75	1.17	1.24
1	C	93	VAL	C-O	-5.74	1.17	1.24
1	B	80	ASP	C-O	-5.74	1.17	1.24
1	A	97	ILE	C-O	-5.72	1.18	1.24
1	A	182	ILE	CA-CB	-5.70	1.51	1.54
1	A	149	THR	C-O	-5.68	1.17	1.23
1	D	97	ILE	C-O	-5.67	1.17	1.24
1	D	77	LYS	C-O	-5.67	1.16	1.24
1	A	235	VAL	C-O	-5.64	1.17	1.24
1	B	224	LYS	C-O	-5.64	1.17	1.23
1	B	239	ILE	C-O	-5.63	1.17	1.24
1	D	94	PHE	C-O	-5.62	1.17	1.24
1	D	59	ASP	C-O	-5.62	1.17	1.24
1	D	69	LYS	C-O	-5.62	1.16	1.24
1	C	229	VAL	C-O	-5.62	1.18	1.24
1	A	74	GLU	C-O	-5.61	1.17	1.24
1	A	169	GLU	C-O	-5.59	1.17	1.24
1	B	9	VAL	C-O	-5.58	1.18	1.24
1	D	202	LEU	C-O	-5.58	1.17	1.23
1	A	118	GLU	C-O	-5.57	1.17	1.24
1	A	90	LEU	C-O	-5.56	1.17	1.24
1	B	133	PHE	C-O	-5.56	1.17	1.24
1	D	24	LEU	C-O	-5.54	1.17	1.24
1	B	90	LEU	C-O	-5.53	1.17	1.24
1	A	113	ALA	C-O	-5.53	1.17	1.24
1	B	173	TRP	C-O	-5.53	1.17	1.24
1	C	116	VAL	C-O	-5.53	1.17	1.24
1	D	114	ARG	C-O	-5.51	1.17	1.24
1	A	111	ASP	C-O	-5.51	1.17	1.24
1	D	137	ALA	C-O	-5.51	1.17	1.24
1	A	241	TYR	C-O	-5.50	1.17	1.24
1	B	88	PRO	C-O	-5.49	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	LEU	C-O	-5.48	1.17	1.24
1	D	116	VAL	C-O	-5.48	1.17	1.24
1	A	54	HIS	C-O	-5.48	1.17	1.24
1	C	220	LEU	C-O	-5.47	1.17	1.24
1	D	68	GLN	C-O	-5.46	1.17	1.24
1	A	73	LEU	C-O	-5.45	1.17	1.24
1	B	3	GLU	C-O	-5.45	1.17	1.24
1	B	61	THR	C-O	-5.45	1.16	1.23
1	B	17	SER	C-O	-5.44	1.17	1.24
1	B	167	LYS	C-O	-5.44	1.17	1.24
1	D	21	GLU	C-O	-5.42	1.17	1.24
1	B	74	GLU	C-O	-5.39	1.17	1.24
1	D	58	ILE	C-O	-5.36	1.18	1.24
1	D	160	VAL	C-O	-5.36	1.18	1.24
1	D	42	VAL	C-O	-5.35	1.18	1.24
1	A	199	SER	C-O	-5.35	1.17	1.24
1	B	237	ARG	C-O	-5.34	1.18	1.24
1	D	50	VAL	C-O	-5.34	1.18	1.24
1	A	65	LYS	C-O	-5.33	1.17	1.23
1	A	87	ILE	C-O	-5.32	1.17	1.24
1	A	21	GLU	C-O	-5.32	1.17	1.23
1	A	134	ASP	C-O	-5.31	1.17	1.24
1	A	153	LEU	C-O	-5.30	1.17	1.23
1	B	121	ALA	CA-CB	-5.29	1.44	1.53
1	D	179	MET	C-O	-5.27	1.17	1.24
1	C	194	LEU	C-O	-5.27	1.18	1.24
1	C	28	ARG	C-O	-5.27	1.18	1.24
1	A	76	LEU	C-O	-5.27	1.18	1.24
1	D	193	ALA	CA-CB	-5.26	1.45	1.53
1	B	235	VAL	C-O	-5.25	1.18	1.24
1	A	163	ILE	C-O	-5.25	1.18	1.24
1	A	208	THR	C-O	-5.25	1.17	1.23
1	A	52	VAL	C-O	-5.25	1.18	1.24
1	A	121	ALA	C-O	-5.25	1.17	1.24
1	A	91	GLU	C-O	-5.24	1.18	1.24
1	D	191	LEU	C-O	-5.24	1.18	1.24
1	D	183	PRO	C-O	-5.23	1.17	1.24
1	B	21	GLU	C-O	-5.23	1.17	1.23
1	A	17	SER	C-O	-5.22	1.18	1.24
1	B	229	VAL	C-O	-5.22	1.18	1.24
1	B	116	VAL	C-O	-5.20	1.18	1.24
1	C	20	PRO	C-N	-5.20	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	LEU	C-O	-5.20	1.18	1.24
1	A	239	ILE	C-O	-5.20	1.18	1.24
1	A	60	ARG	C-O	-5.20	1.18	1.24
1	A	231	ILE	C-O	-5.19	1.18	1.24
1	C	44	LEU	C-O	-5.18	1.17	1.24
1	A	85	GLU	C-O	-5.17	1.17	1.23
1	D	238	MET	C-O	-5.17	1.18	1.24
1	D	177	VAL	CA-CB	-5.16	1.49	1.55
1	A	232	ALA	C-O	-5.15	1.17	1.23
1	D	175	VAL	C-O	-5.15	1.18	1.24
1	A	108	LYS	C-O	-5.14	1.17	1.24
1	C	91	GLU	C-O	-5.14	1.18	1.24
1	A	133	PHE	C-O	-5.14	1.17	1.24
1	D	20	PRO	C-O	-5.14	1.17	1.23
1	B	107	LEU	C-O	-5.13	1.17	1.24
1	A	116	VAL	C-O	-5.13	1.18	1.24
1	D	154	ILE	C-O	-5.13	1.18	1.24
1	D	230	VAL	C-O	-5.13	1.19	1.24
1	C	21	GLU	C-O	-5.12	1.17	1.23
1	D	109	ASP	C-O	-5.12	1.17	1.24
1	C	163	ILE	C-O	-5.11	1.18	1.24
1	C	114	ARG	C-O	-5.11	1.18	1.24
1	C	52	VAL	C-O	-5.10	1.18	1.24
1	A	8	ILE	C-O	-5.09	1.18	1.24
1	D	152	LEU	C-O	-5.08	1.17	1.24
1	D	38	ILE	C-O	-5.07	1.18	1.23
1	B	163	ILE	C-O	-5.06	1.18	1.24
1	A	126	GLU	C-O	-5.06	1.17	1.24
1	B	40	LEU	C-O	-5.06	1.17	1.23
1	A	48	GLY	C-O	-5.05	1.17	1.23
1	D	54	HIS	C-O	-5.05	1.18	1.24
1	C	19	TYR	C-O	-5.05	1.19	1.24
1	A	190	THR	C-O	-5.04	1.18	1.24
1	C	35	ALA	C-O	-5.04	1.17	1.23
1	B	87	ILE	C-O	-5.03	1.18	1.24
1	A	227	PHE	C-O	-5.02	1.17	1.23
1	C	29	LYS	C-O	-5.02	1.18	1.24
1	C	177	VAL	C-O	-5.01	1.18	1.24
1	C	174	SER	C-O	-5.00	1.17	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	N-CA-C	10.04	125.91	112.25
1	D	184	LEU	N-CA-C	7.55	119.30	111.14
1	C	54	HIS	N-CA-C	7.51	119.37	111.03
1	A	54	HIS	N-CA-C	7.47	119.32	111.03
1	C	212	VAL	N-CA-C	-7.06	104.10	111.58
1	A	184	LEU	N-CA-C	6.99	118.69	111.14
1	A	47	ASP	O-C-N	-6.81	111.27	121.63
1	D	54	HIS	N-CA-C	6.57	118.23	111.14
1	B	123	ASN	N-CA-C	6.50	119.20	110.88
1	C	181	ALA	N-CA-C	-6.45	104.29	111.71
1	D	177	VAL	N-CA-C	6.25	115.94	108.45
1	B	184	LEU	N-CA-C	6.22	117.94	111.03
1	C	209	GLU	N-CA-C	6.20	117.70	111.07
1	A	160	VAL	CB-CA-C	-6.12	107.87	114.35
1	C	181	ALA	CA-C-N	-5.85	115.65	120.33
1	C	181	ALA	C-N-CA	-5.85	115.65	120.33
1	C	211	ASP	CB-CA-C	-5.83	100.03	111.06
1	D	204	VAL	N-CA-C	5.71	116.35	108.12
1	D	91	GLU	CA-C-N	5.50	127.64	120.28
1	D	91	GLU	C-N-CA	5.50	127.64	120.28
1	B	160	VAL	CB-CA-C	-5.41	108.62	114.35
1	B	124	ASN	N-CA-C	5.39	121.71	109.81
1	D	211	ASP	CB-CA-C	-5.27	101.10	111.06
1	B	211	ASP	CB-CA-C	-5.25	100.42	110.65
1	A	211	ASP	CB-CA-C	-5.21	101.22	111.06
1	D	235	VAL	N-CA-C	5.20	115.92	110.62
1	C	187	LEU	N-CA-C	5.12	116.55	111.07
1	A	96	ALA	N-CA-C	5.11	118.78	112.54
1	A	154	ILE	N-CA-C	5.09	115.44	108.12
1	B	54	HIS	N-CA-C	5.02	116.61	111.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ASP	Mainchain
1	D	47	ASP	Mainchain

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	2004	0	2044	16	0
1	B	2004	0	2044	27	0
1	C	2004	0	2044	66	0
1	D	2004	0	2044	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	224	0	0	3	0
3	B	185	0	0	2	0
3	C	107	0	0	9	0
3	D	177	0	0	8	0
All	All	8713	0	8176	145	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 9.

All (145) 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:C:187:LEU:CD2	1:C:191:LEU:HD11	1.65	1.27
1:D:99:ARG:HG3	1:D:124:ASN:ND2	1.69	1.07
1:C:187:LEU:CD2	1:C:191:LEU:CD1	2.36	1.03
1:C:187:LEU:HD21	1:C:191:LEU:HD11	1.40	1.02
1:D:99:ARG:HG3	1:D:124:ASN:HD22	1.19	1.01
1:D:99:ARG:CG	1:D:124:ASN:ND2	2.25	0.99
1:C:187:LEU:O	1:C:191:LEU:HD13	1.66	0.94
1:C:99:ARG:HD2	3:C:596:HOH:O	1.66	0.94
1:D:124:ASN:HB3	3:D:575:HOH:O	1.69	0.92
1:C:104:ASN:CG	1:C:129:MET:HE3	1.97	0.90
1:C:187:LEU:HD23	1:C:191:LEU:CD1	2.04	0.86
1:C:187:LEU:HD23	1:C:191:LEU:HD11	1.56	0.84
1:C:114:ARG:HG3	1:C:144:TYR:CZ	2.13	0.84
1:C:114:ARG:HG3	1:C:144:TYR:CE1	2.15	0.81
1:C:188:GLU:H	1:C:188:GLU:CD	1.88	0.81
1:B:165:LYS:HG2	3:B:514:HOH:O	1.79	0.81
1:D:212:VAL:HG13	3:D:517:HOH:O	1.81	0.80
1:D:99:ARG:CG	1:D:124:ASN:HD21	1.94	0.80
1:A:40:LEU:C	1:A:40:LEU:HD12	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASN:O	1:C:211:ASP:HB2	1.82	0.79
1:C:191:LEU:HD12	1:C:191:LEU:N	1.97	0.79
1:D:99:ARG:HD3	3:D:619:HOH:O	1.84	0.78
1:D:182:ILE:HB	1:D:183:PRO:HD3	1.68	0.75
1:B:219:ASN:HA	1:B:222:LYS:HE3	1.67	0.75
1:C:187:LEU:O	1:C:191:LEU:CD1	2.36	0.74
1:C:1:MET:HE1	3:C:599:HOH:O	1.86	0.74
1:D:53:MET:HE3	1:D:58:ILE:HG22	1.68	0.73
1:D:65:LYS:HE3	3:D:625:HOH:O	1.87	0.73
1:D:99:ARG:HG2	1:D:124:ASN:HD21	1.52	0.72
1:B:141:TYR:CE2	1:B:145:ASP:HB3	2.26	0.71
1:C:160:VAL:N	1:C:161:PRO:HD2	2.05	0.70
1:A:28:ARG:NH2	3:A:607:HOH:O	2.25	0.70
1:B:56:GLU:OE2	1:B:67:ARG:NH2	2.24	0.70
1:C:104:ASN:ND2	1:C:129:MET:HE3	2.09	0.68
1:C:187:LEU:O	1:C:187:LEU:HD23	1.94	0.68
1:A:40:LEU:HD12	1:A:40:LEU:O	1.94	0.66
1:C:180:GLU:O	1:C:183:PRO:HD2	1.95	0.65
1:C:156:ARG:HD2	1:C:158:GLU:OE2	1.96	0.65
1:C:191:LEU:CD1	1:C:191:LEU:N	2.60	0.64
1:A:64:MET:HE1	1:A:78:LYS:HB3	1.78	0.64
1:D:124:ASN:CB	3:D:575:HOH:O	2.36	0.64
1:C:180:GLU:N	1:C:180:GLU:OE1	2.30	0.64
1:C:180:GLU:O	1:C:183:PRO:HG2	1.97	0.64
1:C:191:LEU:CD1	1:C:191:LEU:H	2.11	0.63
1:B:78:LYS:HE2	3:C:597:HOH:O	1.99	0.63
1:D:210:ASN:O	1:D:211:ASP:HB2	1.98	0.63
1:C:171:ASN:HB2	3:C:526:HOH:O	1.98	0.62
1:C:187:LEU:HD22	1:C:191:LEU:CD1	2.31	0.61
1:C:187:LEU:CD2	1:C:187:LEU:C	2.74	0.60
1:C:213:LEU:HB2	3:C:502:HOH:O	2.02	0.60
1:B:40:LEU:HD12	1:B:40:LEU:C	2.27	0.60
1:C:213:LEU:HD13	3:C:572:HOH:O	2.01	0.60
1:C:12:HIS:HB2	1:C:231:ILE:HG22	1.84	0.59
1:C:187:LEU:CD2	1:C:191:LEU:HD13	2.33	0.59
1:C:210:ASN:HB2	1:C:212:VAL:HG12	1.84	0.59
1:C:205:VAL:HG22	1:C:229:VAL:HB	1.85	0.58
1:C:236:VAL:O	1:C:240:GLU:HG3	2.04	0.57
1:B:99:ARG:NH1	1:B:124:ASN:HB2	2.19	0.57
1:D:182:ILE:HB	1:D:183:PRO:CD	2.34	0.56
1:C:114:ARG:HG3	1:C:144:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLU:O	1:C:183:PRO:CD	2.54	0.56
1:C:182:ILE:N	1:C:183:PRO:HD2	2.20	0.56
1:B:156:ARG:HH11	1:B:158:GLU:CD	2.14	0.55
1:B:216:LYS:O	1:B:217:ASP:HB2	2.05	0.55
1:B:205:VAL:HG22	1:B:229:VAL:HB	1.89	0.55
1:C:180:GLU:C	1:C:183:PRO:HD2	2.31	0.55
1:C:230:VAL:HG23	1:C:230:VAL:O	2.05	0.55
1:A:40:LEU:C	1:A:40:LEU:CD1	2.76	0.54
1:C:212:VAL:HG13	1:C:213:LEU:N	2.22	0.54
1:D:12:HIS:HE1	3:D:672:HOH:O	1.89	0.54
1:A:142:ARG:HG2	1:A:150:MET:HE1	1.89	0.54
1:A:141:TYR:CE2	1:A:145:ASP:HB3	2.43	0.54
1:A:64:MET:HE1	1:A:78:LYS:CB	2.37	0.53
1:B:46:LYS:HE2	1:B:70:ASP:O	2.08	0.53
1:D:40:LEU:C	1:D:40:LEU:HD12	2.34	0.53
1:C:180:GLU:O	1:C:181:ALA:C	2.49	0.53
1:D:141:TYR:CE2	1:D:145:ASP:HB3	2.44	0.53
1:B:46:LYS:HE2	1:B:70:ASP:C	2.34	0.52
1:C:187:LEU:CD2	1:C:187:LEU:O	2.57	0.52
1:C:114:ARG:CG	1:C:144:TYR:CE1	2.91	0.52
1:C:114:ARG:HG3	1:C:144:TYR:CD1	2.45	0.52
1:D:184:LEU:HD23	1:D:185:ILE:HG23	1.92	0.51
1:C:180:GLU:O	1:C:183:PRO:CG	2.59	0.51
1:C:187:LEU:HD23	1:C:187:LEU:C	2.36	0.51
1:C:188:GLU:CD	1:C:188:GLU:N	2.65	0.51
3:A:573:HOH:O	1:D:115:GLU:HG2	2.10	0.50
1:A:160:VAL:HB	1:A:161:PRO:HD3	1.93	0.50
1:D:99:ARG:CD	3:D:619:HOH:O	2.52	0.50
1:D:216:LYS:O	1:D:217:ASP:HB2	2.11	0.50
1:D:182:ILE:CB	1:D:183:PRO:HD3	2.40	0.50
1:C:40:LEU:HD23	1:C:40:LEU:N	2.27	0.49
1:C:160:VAL:N	1:C:161:PRO:CD	2.74	0.49
1:C:178:PRO:HA	1:C:207:TRP:O	2.13	0.49
1:C:173:TRP:CE3	1:C:174:SER:HB3	2.47	0.49
1:D:54:HIS:HD2	1:D:55:ASP:OD1	1.96	0.49
1:C:248:ARG:HD3	3:C:528:HOH:O	2.12	0.49
1:A:248:ARG:HD2	3:A:525:HOH:O	2.14	0.48
1:C:191:LEU:HD12	1:C:191:LEU:H	1.68	0.48
1:D:158:GLU:O	1:D:161:PRO:HD2	2.14	0.48
1:C:99:ARG:HD3	1:C:127:ARG:NH2	2.30	0.47
1:B:127:ARG:HD2	1:B:127:ARG:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HG2	1:B:170:LEU:HD21	1.97	0.47
1:D:212:VAL:CG1	3:D:517:HOH:O	2.52	0.46
1:B:127:ARG:HD2	1:B:128:VAL:HG23	1.97	0.46
1:B:110:ARG:NH2	1:B:140:GLU:OE1	2.49	0.46
1:A:53:MET:HE3	1:A:58:ILE:HG22	1.97	0.46
1:C:49:ARG:HD3	3:C:578:HOH:O	2.16	0.45
1:D:40:LEU:HD12	1:D:40:LEU:O	2.16	0.45
1:A:54:HIS:HD2	1:A:55:ASP:OD1	1.99	0.45
1:D:72:THR:OG1	1:D:75:GLU:HG3	2.17	0.45
1:B:139:ARG:NH1	1:B:169:GLU:OE2	2.42	0.44
1:D:88:PRO:HA	1:D:92:GLU:OE1	2.16	0.44
1:A:178:PRO:HA	1:A:207:TRP:O	2.17	0.44
1:A:210:ASN:O	1:A:211:ASP:HB2	2.18	0.44
1:D:124:ASN:O	1:D:127:ARG:HG3	2.18	0.44
1:B:234:ASP:C	1:B:234:ASP:OD1	2.61	0.44
1:A:74:GLU:OE1	1:D:143:LYS:NZ	2.49	0.44
1:D:160:VAL:N	1:D:161:PRO:CD	2.81	0.43
1:C:12:HIS:O	1:C:13:ARG:HB2	2.18	0.43
1:C:72:THR:HB	3:C:546:HOH:O	2.17	0.43
1:B:178:PRO:HA	1:B:207:TRP:O	2.18	0.43
1:B:160:VAL:HB	1:B:161:PRO:HD3	2.00	0.43
1:B:160:VAL:N	1:B:161:PRO:CD	2.82	0.43
1:D:194:LEU:O	1:D:198:ARG:HG3	2.18	0.43
1:D:230:VAL:O	1:D:230:VAL:HG23	2.18	0.43
1:C:145:ASP:OD1	1:C:145:ASP:C	2.61	0.42
1:C:187:LEU:HD22	1:C:191:LEU:HD13	1.99	0.42
1:C:141:TYR:CE2	1:C:145:ASP:HB3	2.54	0.42
1:B:46:LYS:CE	1:B:70:ASP:O	2.67	0.42
1:B:210:ASN:O	1:B:211:ASP:HB2	2.19	0.42
1:B:240:GLU:HG2	3:B:587:HOH:O	2.19	0.42
1:C:12:HIS:HD2	1:C:233:ASN:OD1	2.01	0.42
1:B:56:GLU:CD	1:B:67:ARG:HH21	2.24	0.42
1:D:182:ILE:CB	1:D:183:PRO:CD	2.95	0.42
1:C:110:ARG:NH2	1:C:140:GLU:OE1	2.53	0.41
1:C:29:LYS:HD3	1:C:29:LYS:HA	1.93	0.41
1:C:110:ARG:HH11	1:C:110:ARG:HD3	1.73	0.41
1:D:173:TRP:CE3	1:D:174:SER:HB3	2.56	0.41
1:C:114:ARG:HH11	1:C:114:ARG:HD3	1.72	0.41
1:C:210:ASN:HB2	1:C:212:VAL:CG1	2.49	0.41
1:B:35:ALA:HB2	1:B:235:VAL:HG11	2.03	0.40
1:D:101:ALA:O	1:D:127:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:N	1:A:161:PRO:CD	2.84	0.40
1:B:127:ARG:C	1:B:127:ARG:CD	2.94	0.40
1:D:99:ARG:HG2	1:D:124:ASN:ND2	2.13	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	246/248 (99%)	243 (99%)	3 (1%)	0	100	100
1	B	246/248 (99%)	242 (98%)	4 (2%)	0	100	100
1	C	246/248 (99%)	243 (99%)	3 (1%)	0	100	100
1	D	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
All	All	984/992 (99%)	968 (98%)	16 (2%)	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	219/219 (100%)	214 (98%)	5 (2%)	44	40
1	B	219/219 (100%)	216 (99%)	3 (1%)	59	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	219/219 (100%)	212 (97%)	7 (3%)	34	27
1	D	219/219 (100%)	214 (98%)	5 (2%)	44	40
All	All	876/876 (100%)	856 (98%)	20 (2%)	44	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	40	LEU
1	A	65	LYS
1	A	115	GLU
1	A	162	LEU
1	B	127	ARG
1	B	218	ASP
1	B	235	VAL
1	C	122	GLU
1	C	159	VAL
1	C	187	LEU
1	C	188	GLU
1	C	192	GLN
1	C	224	LYS
1	C	235	VAL
1	D	4	ARG
1	D	40	LEU
1	D	99	ARG
1	D	184	LEU
1	D	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	123	ASN
1	B	104	ASN
1	B	210	ASN
1	C	12	HIS
1	C	54	HIS
1	C	83	GLN
1	D	12	HIS
1	D	54	HIS

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Mol	Chain	Res	Type
1	D	104	ASN
1	D	124	ASN
1	D	192	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	248/248 (100%)	-0.17	0 100 100	17, 24, 36, 42	0
1	B	248/248 (100%)	-0.04	0 100 100	18, 26, 38, 46	0
1	C	248/248 (100%)	0.46	4 (1%) 70 74	24, 35, 52, 62	0
1	D	248/248 (100%)	-0.03	1 (0%) 88 90	16, 27, 40, 46	0
All	All	992/992 (100%)	0.06	5 (0%) 87 89	16, 28, 44, 62	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	184	LEU	4.0
1	C	187	LEU	2.7
1	D	124	ASN	2.3
1	C	241	TYR	2.3
1	C	181	ALA	2.3

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(Å ²)	Q<0.9
2	MG	B	401	1/1	0.90	0.07	24,24,24,24	0
2	MG	C	401	1/1	0.90	0.06	30,30,30,30	0
2	MG	D	401	1/1	0.95	0.04	20,20,20,20	0
2	MG	A	401	1/1	0.98	0.04	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.