



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:44 AM UTC

PDB ID : 4LEF / pdb_00004lef
Title : Crystal structure of PHOSPHOTRIESTERASE HOMOLOGY PROTEIN
FROM ESCHERICHIA COLI complexed with phosphate in active site
Authors : Fedorov, A.A.; Fedorov, E.V.; Xiang, D.F.; Raushel, F.M.; Almo, S.C.
Deposited on : 2013-06-25
Resolution : 1.84 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)
Validation Pipeline (wwPDB-VP) : 2.49

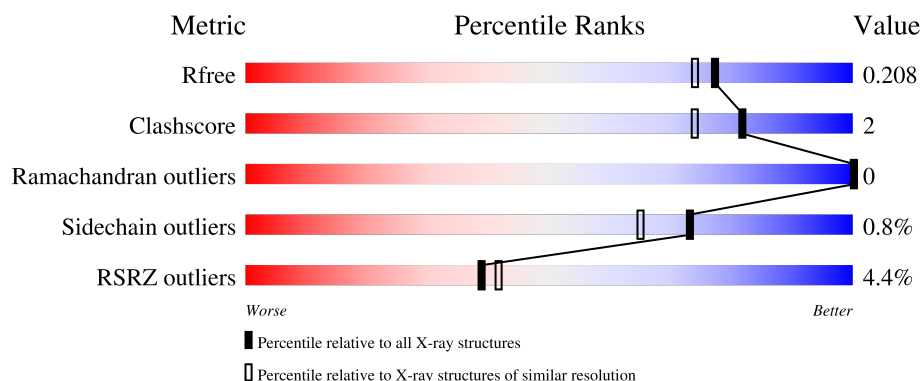
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	292	94% 5%
1	B	292	% 95% ..
1	C	292	% 91% 8% .
1	D	292	3% 90% 10% .
1	E	292	2% 92% 8% .

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Mol	Chain	Length	Quality of chain
1	F	292	% 93% 6%
1	G	292	2% 95% 5%
1	H	292	26% 92% 7% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20380 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 Phosphotriesterase homology protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	290	Total	C	N	O	S	0	1	0
			2308	1445	402	442	19			
1	D	290	Total	C	N	O	S	0	0	0
			2292	1435	400	440	17			
1	A	291	Total	C	N	O	S	0	3	0
			2325	1453	408	446	18			
1	B	290	Total	C	N	O	S	0	3	0
			2319	1452	406	443	18			
1	E	290	Total	C	N	O	S	0	1	0
			2303	1441	404	441	17			
1	F	291	Total	C	N	O	S	0	2	0
			2315	1448	404	445	18			
1	G	291	Total	C	N	O	S	0	1	0
			2306	1443	402	443	18			
1	H	290	Total	C	N	O	S	0	1	0
			2300	1440	401	441	18			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

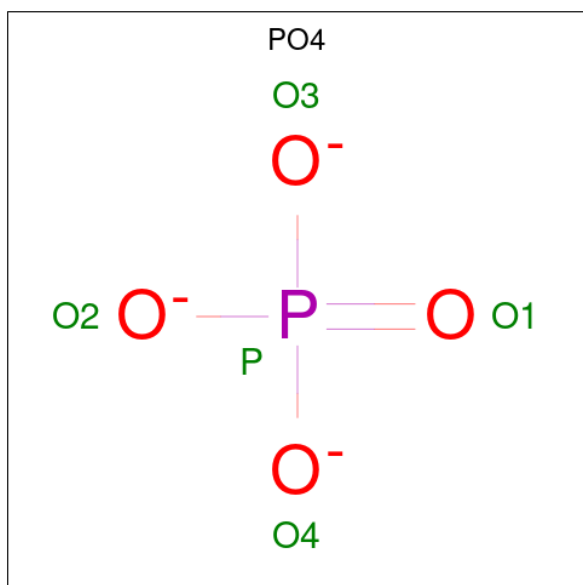
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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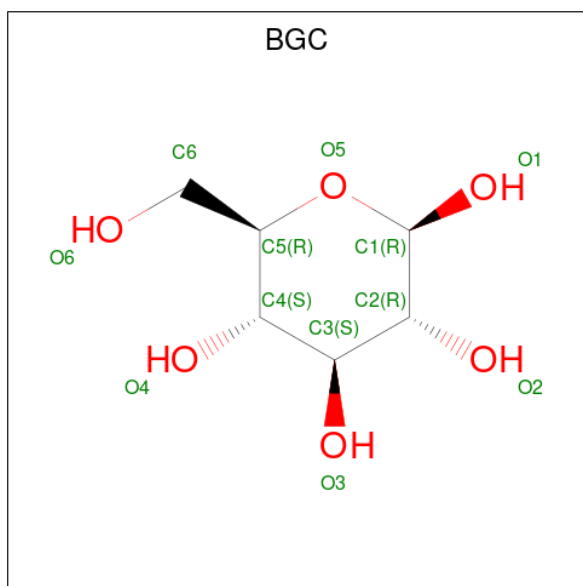
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	248	Total	O	0	1
			249	249		
5	D	198	Total	O	0	1
			199	199		
5	A	283	Total	O	0	3
			286	286		
5	B	261	Total	O	0	1
			262	262		
5	E	186	Total	O	0	1
			187	187		
5	F	258	Total	O	0	2
			260	260		
5	G	151	Total	O	0	1
			152	152		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	134	Total 134	O 134	0	0

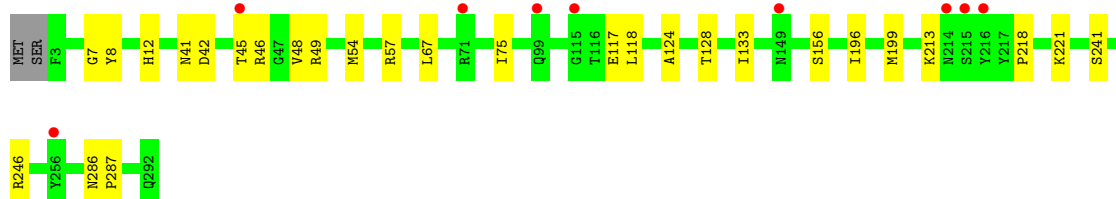
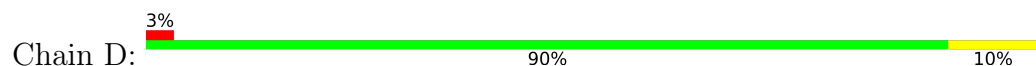
3 Residue-property plots [i](#)

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: Phosphotriesterase homology protein



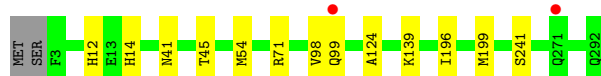
- Molecule 1: Phosphotriesterase homology protein



- Molecule 1: Phosphotriesterase homology protein



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- Molecule 1: Phosphotriesterase homology protein

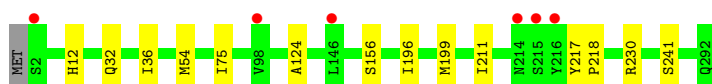




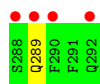
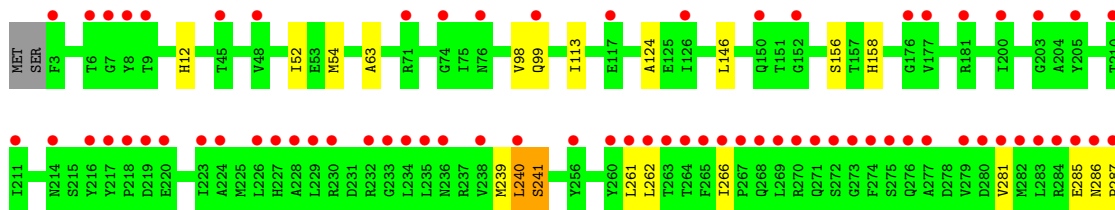
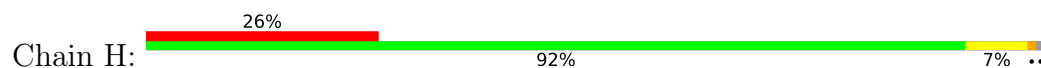
- Molecule 1: Phosphotriesterase homology protein



- Molecule 1: Phosphotriesterase homology protein



- Molecule 1: Phosphotriesterase homology protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.05Å 100.31Å 168.04Å 90.00° 104.48° 90.00°	Depositor
Resolution (Å)	42.57 – 1.84 42.57 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.57-1.84) 99.2 (42.57-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.175 , 0.208 0.175 , 0.208	Depositor DCC
R_{free} test set	6885 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20380	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5965e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, ZN, PO4

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	0.49	0/2365	0.75	0/3191
1	B	0.48	0/2359	0.77	0/3183
1	C	0.47	0/2348	0.75	0/3168
1	D	0.43	0/2332	0.73	0/3148
1	E	0.44	0/2343	0.73	0/3162
1	F	0.49	0/2355	0.75	0/3178
1	G	0.41	0/2346	0.72	0/3166
1	H	0.44	2/2340 (0.1%)	0.77	3/3158 (0.1%)
All	All	0.46	2/18788 (0.0%)	0.74	3/25354 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	239	MET	C-N	-6.24	1.25	1.33
1	H	240	LEU	C-N	5.27	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	239	MET	CA-C-N	-6.78	110.02	121.75
1	H	239	MET	C-N-CA	-6.78	110.02	121.75
1	H	240	LEU	O-C-N	-5.11	117.42	123.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124	ALA	Peptide

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	2325	0	2271	9	0
1	B	2319	0	2271	9	0
1	C	2308	0	2258	13	0
1	D	2292	0	2241	15	0
1	E	2303	0	2253	12	0
1	F	2315	0	2261	12	0
1	G	2306	0	2254	5	0
1	H	2300	0	2249	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	20	0	0	0	0
3	B	25	0	0	1	0
3	C	15	0	0	0	0
3	D	20	0	0	2	0
3	E	20	0	0	0	0
3	F	20	0	0	0	0
3	G	20	0	0	0	0
3	H	15	0	0	0	0
4	B	12	0	11	0	0
5	A	286	0	0	0	0
5	B	262	0	0	4	0
5	C	249	0	0	0	0
5	D	199	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	187	0	0	0	0
5	F	260	0	0	2	0
5	G	152	0	0	0	0
5	H	134	0	0	2	0
All	All	20380	0	18069	90	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 2.

All (90) 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:E:217:TYR:CZ	1:E:221:LYS:HB3	2.32	0.65
1:H:99:GLN:NE2	5:H:509:HOH:O	2.30	0.65
1:E:46[B]:ARG:NH1	1:E:259:ASP:OD2	2.29	0.65
1:C:48:VAL:HG23	1:C:262:LEU:HD11	1.83	0.61
1:H:240:LEU:HD23	1:H:241:SER:N	2.16	0.60
1:H:281:VAL:HA	1:H:285:GLU:HB2	1.85	0.59
1:C:68:ASP:OD1	1:C:71:ARG:NH2	2.35	0.58
1:E:196:ILE:HA	1:E:199:MET:HE3	1.84	0.58
1:D:67:LEU:HD21	1:D:118:LEU:HB2	1.88	0.56
1:C:218:PRO:HG2	1:C:221:LYS:HG3	1.88	0.56
1:F:40:MET:O	1:F:44[B]:MET:HG3	2.06	0.55
1:F:71:ARG:NH1	5:F:610:HOH:O	2.39	0.54
1:C:124:ALA:HB2	1:C:156:SER:HB3	1.90	0.53
1:G:196:ILE:HA	1:G:199:MET:HE3	1.90	0.52
1:H:124:ALA:HB2	1:H:156:SER:HB3	1.92	0.52
1:C:12:HIS:CG	1:C:54:MET:HG3	2.45	0.51
1:A:41:ASN:O	1:A:45:THR:HG23	2.10	0.51
1:A:12:HIS:CG	1:A:54:MET:HG3	2.45	0.51
1:D:57:ARG:NH1	3:D:306:PO4:O3	2.40	0.51
1:H:12:HIS:CG	1:H:54:MET:HG3	2.46	0.50
1:F:48:VAL:HG23	1:F:262:LEU:HD11	1.94	0.50
1:B:196:ILE:HA	1:B:199:MET:HE3	1.94	0.50
1:D:42:ASP:O	1:D:46:ARG:HG2	2.12	0.49
1:G:124:ALA:HB2	1:G:156:SER:HB3	1.93	0.49
1:F:12:HIS:CG	1:F:54:MET:HG3	2.48	0.49
1:G:12:HIS:CG	1:G:54:MET:HG3	2.48	0.49
1:H:240:LEU:HD22	1:H:261:LEU:HD21	1.94	0.49
1:H:262:LEU:HD23	1:H:266:ILE:HG13	1.95	0.48
1:B:98:VAL:HG22	1:B:139:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:HIS:CG	1:D:54:MET:HG3	2.48	0.48
1:F:277:ALA:O	1:F:281:VAL:HG23	2.12	0.48
1:A:196:ILE:HA	1:A:199:MET:HE3	1.96	0.48
1:D:8:TYR:HB2	1:D:48:VAL:HA	1.97	0.47
1:D:246:ARG:NE	3:D:304:PO4:O2	2.44	0.47
1:E:12:HIS:CG	1:E:54:MET:HG3	2.50	0.47
1:F:124:ALA:HB2	1:F:156:SER:HB3	1.97	0.47
1:D:218:PRO:HG2	1:D:221:LYS:HG3	1.95	0.47
1:G:32:GLN:O	1:G:36:ILE:HG12	2.14	0.47
1:D:12:HIS:CD2	1:D:54:MET:HG3	2.50	0.47
1:F:196:ILE:HA	1:F:199:MET:HE3	1.96	0.47
1:E:218:PRO:HG2	1:E:221:LYS:HD3	1.97	0.46
1:H:12:HIS:CD2	1:H:54:MET:HG3	2.50	0.46
1:B:12:HIS:CG	1:B:54:MET:HG3	2.50	0.46
1:A:124:ALA:HB2	1:A:156:SER:HB3	1.96	0.46
1:B:98:VAL:HG23	5:B:463:HOH:O	2.13	0.46
1:A:117:GLU:H	1:A:117:GLU:CD	2.23	0.46
1:C:41:ASN:O	1:C:45:THR:HG23	2.15	0.46
1:E:124:ALA:HB2	1:E:156:SER:HB3	1.98	0.46
1:E:41:ASN:O	1:E:45:THR:HG23	2.16	0.46
1:H:240:LEU:CD2	1:H:261:LEU:CD2	2.95	0.45
1:F:12:HIS:CD2	1:F:54:MET:HG3	2.50	0.45
1:C:98:VAL:HG22	1:C:139:LYS:HG3	1.99	0.45
1:E:46[A]:ARG:CZ	1:E:263:THR:HG22	2.47	0.45
1:E:98:VAL:HG11	1:E:142:ILE:HG22	1.98	0.45
1:D:286:ASN:HB2	1:D:287:PRO:HD3	1.99	0.44
1:D:41:ASN:O	1:D:45:THR:HG23	2.17	0.44
1:C:65:PHE:O	1:C:69:VAL:HG23	2.17	0.44
1:B:71[A]:ARG:NH2	5:B:418:HOH:O	2.51	0.44
1:A:128:THR:HG21	1:A:133:ILE:HG12	2.00	0.43
1:C:12:HIS:CD2	1:C:54:MET:HG3	2.53	0.43
3:B:305:PO4:O1	5:B:526:HOH:O	2.21	0.43
1:H:98:VAL:HG12	1:H:146:LEU:HD12	2.00	0.43
1:D:213:LYS:NZ	5:D:557:HOH:O	2.46	0.43
1:F:217:TYR:HA	1:F:218:PRO:HD3	1.86	0.43
1:B:99:GLN:HG3	5:B:657:HOH:O	2.18	0.43
1:E:4:ASP:HA	1:E:5:PRO:HD3	1.80	0.43
1:H:52:ILE:HG22	1:H:54:MET:HE3	2.01	0.43
1:G:217:TYR:HA	1:G:218:PRO:HD3	1.87	0.43
1:A:286:ASN:HB2	1:A:287:PRO:HD3	2.00	0.42
1:A:122:ILE:HD11	1:A:156:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:ALA:HB2	1:H:113:ILE:HG13	2.01	0.42
1:C:286:ASN:HB2	1:C:287:PRO:HD3	2.01	0.42
1:A:146:LEU:HA	1:A:146:LEU:HD23	1.77	0.42
1:B:41:ASN:O	1:B:45:THR:HG23	2.18	0.42
1:H:289:GLN:HG2	5:H:530:HOH:O	2.19	0.42
1:D:124:ALA:HB2	1:D:156:SER:HB3	2.01	0.42
1:D:196:ILE:HA	1:D:199:MET:HE3	2.02	0.42
1:F:52:ILE:HG22	1:F:54:MET:HE3	2.01	0.42
1:C:52:ILE:HG22	1:C:54:MET:HE3	2.01	0.41
1:D:128:THR:HG21	1:D:133:ILE:HG12	2.01	0.41
1:F:43:LEU:HB3	1:F:48:VAL:HB	2.03	0.41
1:E:286:ASN:HB2	1:E:287:PRO:HD3	2.02	0.41
1:D:7:GLY:HA3	1:D:49:ARG:HG3	2.03	0.41
1:B:14:HIS:CE1	1:B:54:MET:HB2	2.56	0.41
1:E:266:ILE:HD13	1:E:266:ILE:HA	1.88	0.40
1:F:71:ARG:NH2	5:F:548:HOH:O	2.54	0.40
1:B:12:HIS:CD2	1:B:54:MET:HG3	2.56	0.40
1:H:286:ASN:HB2	1:H:287:PRO:HD3	2.02	0.40
1:C:14:HIS:CE1	1:C:54:MET:HB2	2.56	0.40
1:C:15:LEU:O	1:C:36:ILE:HD13	2.22	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	292/292 (100%)	287 (98%)	5 (2%)	0	100	100
1	B	291/292 (100%)	284 (98%)	7 (2%)	0	100	100
1	C	290/292 (99%)	284 (98%)	6 (2%)	0	100	100
1	D	288/292 (99%)	280 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	289/292 (99%)	283 (98%)	6 (2%)	0	100	100
1	F	291/292 (100%)	285 (98%)	6 (2%)	0	100	100
1	G	290/292 (99%)	282 (97%)	8 (3%)	0	100	100
1	H	289/292 (99%)	281 (97%)	8 (3%)	0	100	100
All	All	2320/2336 (99%)	2266 (98%)	54 (2%)	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	252/250 (101%)	251 (100%)	1 (0%)	84	78
1	B	251/250 (100%)	250 (100%)	1 (0%)	84	78
1	C	250/250 (100%)	248 (99%)	2 (1%)	73	65
1	D	248/250 (99%)	245 (99%)	3 (1%)	63	51
1	E	249/250 (100%)	248 (100%)	1 (0%)	84	78
1	F	251/250 (100%)	250 (100%)	1 (0%)	84	78
1	G	250/250 (100%)	246 (98%)	4 (2%)	55	39
1	H	249/250 (100%)	247 (99%)	2 (1%)	73	65
All	All	2000/2000 (100%)	1985 (99%)	15 (1%)	73	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	10	LEU
1	C	241	SER
1	D	75	ILE
1	D	117	GLU
1	D	241	SER
1	A	241	SER

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Mol	Chain	Res	Type
1	B	241	SER
1	E	241	SER
1	F	241	SER
1	G	75	ILE
1	G	211	ILE
1	G	230	ARG
1	G	241	SER
1	H	158	HIS
1	H	241	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	76	ASN
1	C	150	GLN
1	C	207	GLN
1	D	32	GLN
1	D	253	ASN
1	B	173	GLN
1	B	292	GLN
1	E	207	GLN
1	F	76	ASN
1	F	103	GLN
1	F	207	GLN
1	G	32	GLN
1	G	253	ASN
1	H	32	GLN
1	H	76	ASN
1	H	214	ASN
1	H	253	ASN
1	H	292	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 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	PO4	G	306	-	4,4,4	0.91	0	6,6,6	0.47	0
3	PO4	C	305	-	4,4,4	0.92	0	6,6,6	0.47	0
3	PO4	E	306	-	4,4,4	0.96	0	6,6,6	0.37	0
3	PO4	D	305	-	4,4,4	0.90	0	6,6,6	0.54	0
3	PO4	B	306	-	4,4,4	0.93	0	6,6,6	0.48	0
3	PO4	C	303	2	4,4,4	1.02	0	6,6,6	0.88	0
3	PO4	B	305	-	4,4,4	0.95	0	6,6,6	0.50	0
3	PO4	E	305	-	4,4,4	0.90	0	6,6,6	0.48	0
3	PO4	B	307	-	4,4,4	0.93	0	6,6,6	0.49	0
3	PO4	F	304	-	4,4,4	0.85	0	6,6,6	0.55	0
3	PO4	C	304	-	4,4,4	1.00	0	6,6,6	0.50	0
3	PO4	D	304	-	4,4,4	0.92	0	6,6,6	0.50	0
3	PO4	E	303	2	4,4,4	1.29	1 (25%)	6,6,6	0.50	0
3	PO4	H	303	2	4,4,4	1.03	0	6,6,6	0.58	0
3	PO4	A	306	-	4,4,4	0.91	0	6,6,6	0.44	0
3	PO4	G	303	2	4,4,4	0.96	0	6,6,6	0.54	0
3	PO4	E	304	-	4,4,4	0.88	0	6,6,6	0.55	0
3	PO4	F	305	-	4,4,4	0.94	0	6,6,6	0.45	0
3	PO4	H	304	-	4,4,4	0.91	0	6,6,6	0.66	0
3	PO4	A	304	-	4,4,4	1.14	0	6,6,6	0.48	0
4	BGC	B	308	-	12,12,12	2.11	5 (41%)	17,17,17	1.34	4 (23%)
3	PO4	A	305	-	4,4,4	0.87	0	6,6,6	0.58	0
3	PO4	G	304	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	F	306	-	4,4,4	0.93	0	6,6,6	0.45	0
3	PO4	B	303	2	4,4,4	1.07	0	6,6,6	0.36	0
3	PO4	D	303	2	4,4,4	1.15	0	6,6,6	0.76	0
3	PO4	A	303	2	4,4,4	0.99	0	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	B	304	-	4,4,4	0.90	0	6,6,6	0.47	0
3	PO4	H	305	-	4,4,4	0.90	0	6,6,6	0.52	0
3	PO4	G	305	-	4,4,4	0.94	0	6,6,6	0.44	0
3	PO4	F	303	2	4,4,4	0.98	0	6,6,6	0.70	0
3	PO4	D	306	-	4,4,4	0.86	0	6,6,6	0.44	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
4	BGC	B	308	-	-	0/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	308	BGC	C6-C5	-3.49	1.40	1.51
4	B	308	BGC	O5-C5	3.30	1.52	1.44
4	B	308	BGC	C3-C2	-3.25	1.43	1.52
4	B	308	BGC	C4-C3	-2.55	1.45	1.52
4	B	308	BGC	C1-C2	-2.20	1.47	1.52
3	E	303	PO4	P-O4	-2.03	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	308	BGC	C3-C4-C5	2.26	114.34	110.23
4	B	308	BGC	O5-C5-C4	-2.18	105.77	109.70
4	B	308	BGC	C1-O5-C5	-2.14	109.51	113.65
4	B	308	BGC	O6-C6-C5	2.11	118.50	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	305	PO4	1	0
3	D	304	PO4	1	0
3	D	306	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	291/292 (99%)	-0.64	1 (0%)	90 94	7, 15, 26, 45	3 (1%)
1	B	290/292 (99%)	-0.60	2 (0%)	84 90	4, 16, 31, 40	3 (1%)
1	C	290/292 (99%)	-0.53	2 (0%)	84 90	5, 18, 32, 76	1 (0%)
1	D	290/292 (99%)	0.06	9 (3%)	51 56	12, 28, 47, 84	0
1	E	290/292 (99%)	-0.18	5 (1%)	69 77	14, 25, 39, 81	1 (0%)
1	F	291/292 (99%)	-0.56	3 (1%)	79 86	8, 16, 30, 80	2 (0%)
1	G	291/292 (99%)	0.06	6 (2%)	63 71	12, 29, 50, 97	1 (0%)
1	H	290/292 (99%)	1.07	75 (25%)	1 1	18, 42, 76, 89	1 (0%)
All	All	2323/2336 (99%)	-0.17	103 (4%)	39 42	4, 22, 51, 97	12 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	281	VAL	6.9
1	E	216	TYR	6.4
1	F	216	TYR	6.3
1	G	216	TYR	6.3
1	H	277	ALA	6.2
1	D	216	TYR	5.1
1	H	216	TYR	5.1
1	H	279	VAL	5.0
1	C	216	TYR	4.8
1	H	234	LEU	4.7
1	H	274	PHE	4.5
1	H	266	ILE	4.3
1	H	228	ALA	4.0
1	H	256	TYR	3.9
1	H	269	LEU	3.8
1	H	227	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	8	TYR	3.6
1	H	150	GLN	3.4
1	H	267	PRO	3.4
1	H	240	LEU	3.3
1	H	45	THR	3.3
1	H	283	LEU	3.2
1	H	3	PHE	3.2
1	E	214	ASN	3.2
1	H	224	ALA	3.1
1	H	235	LEU	3.1
1	H	275	SER	3.1
1	G	2	SER	3.0
1	H	205	TYR	3.0
1	C	215	SER	3.0
1	H	270	ARG	3.0
1	H	223	ILE	3.0
1	H	280	ASP	2.9
1	H	264	THR	2.9
1	H	285	GLU	2.9
1	H	230	ARG	2.9
1	H	48	VAL	2.9
1	H	290	PHE	2.9
1	H	238	VAL	2.8
1	H	219	ASP	2.8
1	H	262	LEU	2.8
1	H	233	GLY	2.8
1	H	218	PRO	2.8
1	H	226	LEU	2.8
1	H	289	GLN	2.8
1	H	71	ARG	2.7
1	H	276	GLN	2.7
1	E	71	ARG	2.7
1	H	263	THR	2.7
1	D	215	SER	2.6
1	H	286	ASN	2.6
1	H	152	GLY	2.6
1	H	217	TYR	2.6
1	H	272	SER	2.6
1	H	288	SER	2.6
1	H	211	ILE	2.6
1	H	203	GLY	2.6
1	H	260	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	268	GLN	2.6
1	E	201	ASP	2.6
1	H	265	PHE	2.5
1	H	200	ILE	2.4
1	H	229	LEU	2.4
1	H	214	ASN	2.4
1	D	256	TYR	2.3
1	D	45	THR	2.3
1	D	214	ASN	2.3
1	H	7	GLY	2.3
1	F	2	SER	2.3
1	H	232	ARG	2.3
1	H	126	ILE	2.3
1	H	74	GLY	2.3
1	B	271	GLN	2.3
1	H	271	GLN	2.3
1	H	292	GLN	2.3
1	G	146	LEU	2.3
1	H	282	MET	2.3
1	H	181	ARG	2.3
1	G	215	SER	2.3
1	H	210	THR	2.3
1	G	214	ASN	2.2
1	G	98	VAL	2.2
1	A	2	SER	2.2
1	H	9	THR	2.2
1	D	115	GLY	2.2
1	D	149	ASN	2.1
1	H	177	VAL	2.1
1	H	284	ARG	2.1
1	H	220	GLU	2.1
1	H	236	ASN	2.1
1	D	99	GLN	2.1
1	F	215	SER	2.1
1	H	273	GLY	2.1
1	H	99	GLN	2.1
1	E	46[A]	ARG	2.1
1	B	99	GLN	2.1
1	D	71	ARG	2.1
1	H	176	GLY	2.0
1	H	261	LEU	2.0
1	H	117	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	6	THR	2.0
1	H	76	ASN	2.0
1	H	287	PRO	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(Å ²)	Q<0.9
3	PO4	E	306	5/5	0.52	0.18	83,84,87,87	0
3	PO4	D	306	5/5	0.67	0.13	64,64,68,71	0
3	PO4	A	305	5/5	0.69	0.14	70,72,75,77	0
3	PO4	F	306	5/5	0.70	0.12	90,91,92,93	0
3	PO4	G	306	5/5	0.70	0.17	79,82,84,87	0
3	PO4	G	305	5/5	0.75	0.12	84,84,84,85	0
3	PO4	D	305	5/5	0.76	0.16	83,86,86,89	0
3	PO4	G	304	5/5	0.76	0.15	80,82,83,86	0
3	PO4	B	307	5/5	0.77	0.19	84,86,87,87	0
3	PO4	D	304	5/5	0.78	0.16	77,79,81,82	0
3	PO4	B	305	5/5	0.78	0.14	66,71,72,75	0
3	PO4	C	304	5/5	0.81	0.17	68,73,76,79	0
3	PO4	E	304	5/5	0.82	0.13	63,71,72,74	0
3	PO4	F	305	5/5	0.82	0.12	72,73,74,75	0
3	PO4	C	305	5/5	0.83	0.11	70,72,75,76	0
3	PO4	H	305	5/5	0.83	0.11	69,70,75,75	0
3	PO4	E	305	5/5	0.84	0.13	74,75,78,78	0
3	PO4	A	306	5/5	0.85	0.10	59,62,66,66	0
3	PO4	B	306	5/5	0.85	0.10	66,70,72,72	0
3	PO4	H	304	5/5	0.85	0.13	60,62,64,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	F	304	5/5	0.85	0.12	53,54,64,65	0
3	PO4	B	304	5/5	0.95	0.07	29,35,38,46	0
4	BGC	B	308	12/12	0.95	0.06	10,15,17,26	0
3	PO4	A	304	5/5	0.96	0.07	21,23,30,36	0
2	ZN	H	302	1/1	0.97	0.04	21,21,21,21	0
2	ZN	H	301	1/1	0.98	0.03	21,21,21,21	0
2	ZN	D	301	1/1	0.98	0.02	15,15,15,15	0
3	PO4	D	303	5/5	0.98	0.04	14,15,17,21	0
3	PO4	H	303	5/5	0.98	0.05	20,20,27,31	0
3	PO4	E	303	5/5	0.98	0.05	12,20,22,25	0
3	PO4	A	303	5/5	0.98	0.05	11,13,18,19	0
3	PO4	G	303	5/5	0.98	0.06	19,19,21,21	0
2	ZN	E	302	1/1	0.99	0.02	16,16,16,16	0
2	ZN	G	302	1/1	0.99	0.02	18,18,18,18	0
3	PO4	F	303	5/5	0.99	0.04	10,10,18,19	0
2	ZN	D	302	1/1	0.99	0.02	14,14,14,14	0
2	ZN	E	301	1/1	0.99	0.02	17,17,17,17	0
3	PO4	C	303	5/5	0.99	0.04	8,13,16,18	0
3	PO4	B	303	5/5	0.99	0.04	11,14,18,19	0
2	ZN	G	301	1/1	1.00	0.01	16,16,16,16	0
2	ZN	A	301	1/1	1.00	0.01	10,10,10,10	0
2	ZN	A	302	1/1	1.00	0.01	10,10,10,10	0
2	ZN	B	301	1/1	1.00	0.02	10,10,10,10	0
2	ZN	B	302	1/1	1.00	0.03	12,12,12,12	0
2	ZN	C	301	1/1	1.00	0.01	11,11,11,11	0
2	ZN	C	302	1/1	1.00	0.02	12,12,12,12	0
2	ZN	F	301	1/1	1.00	0.02	10,10,10,10	0
2	ZN	F	302	1/1	1.00	0.01	11,11,11,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.