



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:33 PM UTC

PDB ID : 2F1D / pdb_00002f1d
Title : X-Ray Structure of imidazoglycerol-phosphate dehydratase
Authors : Rice, D.W.; Glynn, S.E.; Baker, P.J.; Sedelnikova, S.E.; Davies, C.L.; Eadsforth, T.C.
Deposited on : 2005-11-14
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

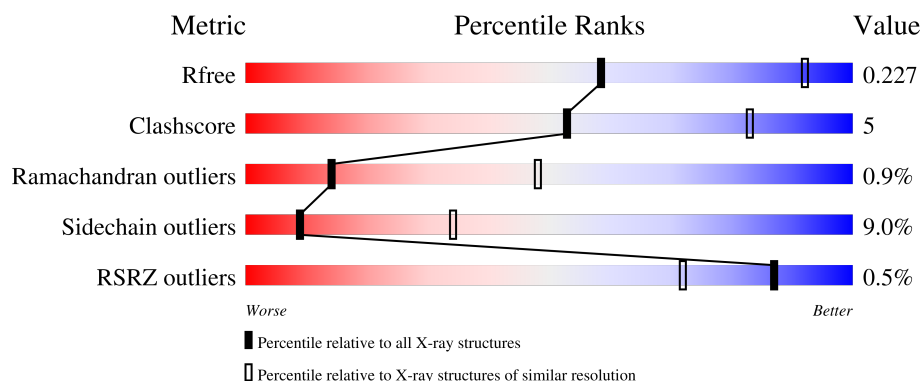
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	207	 71% 15% • 12%
1	B	207	 70% 19% 12%
1	C	207	 72% 15% • 12%
1	D	207	 76% 11% • 12%
1	E	207	 72% 14% • 12%

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Mol	Chain	Length	Quality of chain
1	F	207	% 73% 13% 12%
1	G	207	76% 12% 12%
1	H	207	72% 15% 12%
1	I	207	71% 14% 12%
1	J	207	73% 14% 12%
1	K	207	70% 17% 12%
1	L	207	% 72% 15% 12%
1	M	207	70% 16% 12%
1	N	207	% 71% 16% 12%
1	O	207	% 68% 20% 12%
1	P	207	68% 17% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22288 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 Imidazoleglycerol-phosphate dehydratase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	B	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	C	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	D	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	E	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	F	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	G	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	H	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	I	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	J	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	K	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	L	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	M	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	N	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	O	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			
1	P	183	Total	C	N	O	S	0	0	0
			1386	866	250	268	2			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0
2	C	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0
2	G	2	Total 2	Mn 2	0	0
2	H	2	Total 2	Mn 2	0	0
2	I	2	Total 2	Mn 2	0	0
2	J	2	Total 2	Mn 2	0	0
2	K	2	Total 2	Mn 2	0	0
2	L	2	Total 2	Mn 2	0	0
2	M	2	Total 2	Mn 2	0	0
2	N	2	Total 2	Mn 2	0	0
2	O	2	Total 2	Mn 2	0	0
2	P	2	Total 2	Mn 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		

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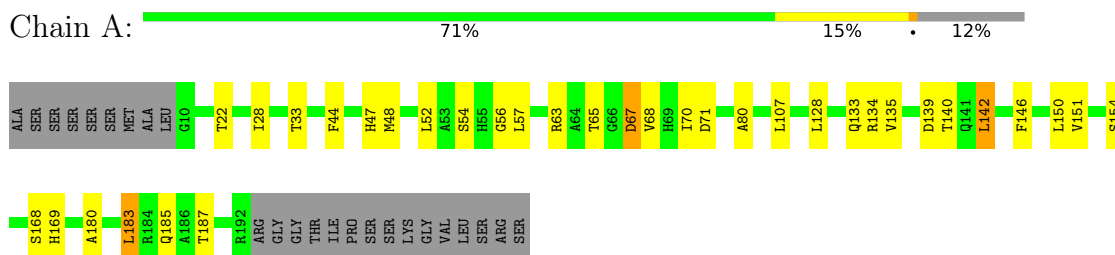
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		

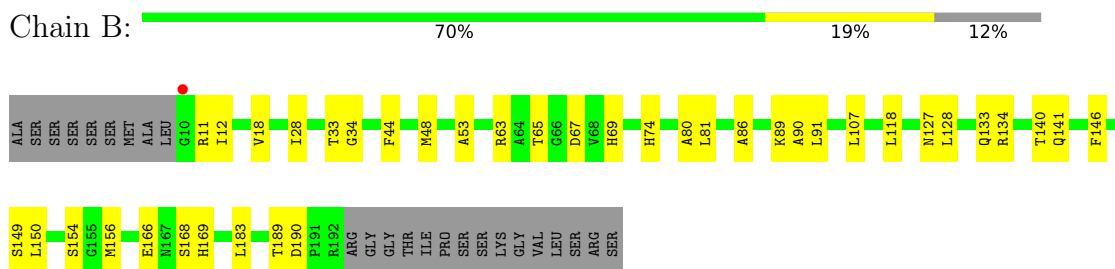
3 Residue-property plots

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.

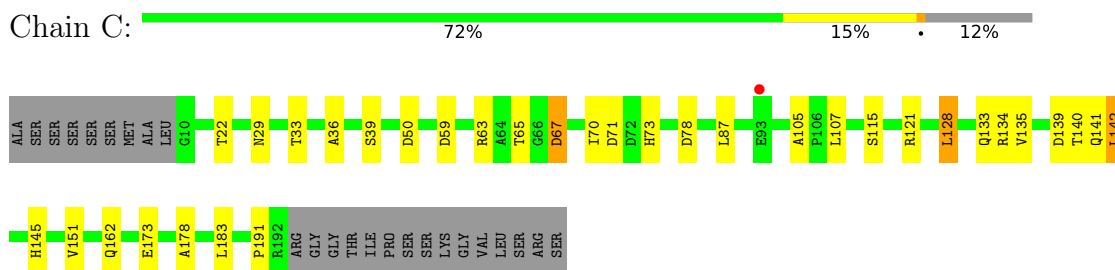
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



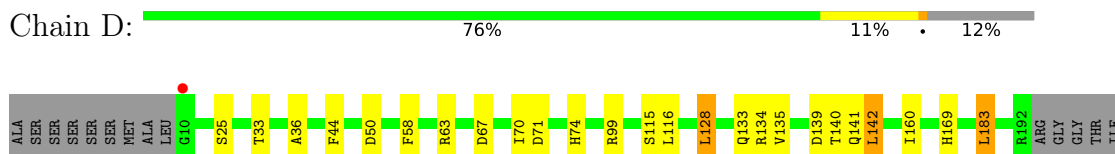
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



PRO
SER
SER
LYS
SER
GLY
VAL
LEU
SER
ARG
SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain E:  72% 14% 12%

ALA SER SER SER SER MET ALA LEU G10 E14 T53 D37 F44 H61 V62 R63 A64 T65 G66 D67 V68 H69 A80 A105 P106 L107 V114 P122 L128 Q133 R134 V135 D139 T140 Q141 L142 F146 M156 Q162 H169 A174

A178 F179 L183 D190 P191 R192 ARG GLY THR ILE PRO SER SER LYS VAL LEU SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain F:  % 73% 13% 12%

ALA SER SER SER SER MET ALA LEU G10 V18 N23 T33 F44 H47 Q51 R63 A64 T65 G66 D67 H73 K89 E93 R94 N98 R99 V114 L128 Q133 R134 D139 T140 Q141 L142 H145 L150 S154 I160 E166

H167 S168 H169 F179 L183 D190 P191 R192 ARG GLY THR ILE PRO SER LYS VAL LEU SER ARG SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain G:  76% 12% 12%

ALA SER SER SER SER MET ALA LEU G10 L30 T33 A36 H47 D60 R63 D67 V68 H69 H73 L81 R89 L116 D117 L118 Q133 R134 V135 T140 Q141 L142 H145 S149 L150 V151 S168 L183 T187 R192 ARG GLY

GLY THR ILE PRO SER SER LYS VAL LEU SER ARG SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain H:  72% 15% 12%

ALA SER SER SER SER MET ALA LEU G10 I12 E21 S25 N29 T33 D37 F44 D59 V60 H61 V62 R63 D67 V68 H69 I70 L107 V114 S115 L116 L128 Q133 R134 D139 T140 Q141 L142 L150 S154 E166 H167 S168 H169

A174 F179 L183 D190 P191 R192 ARG GLY THR ILE PRO SER SER LYS VAL LEU SER ARG SER

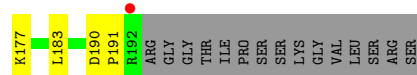
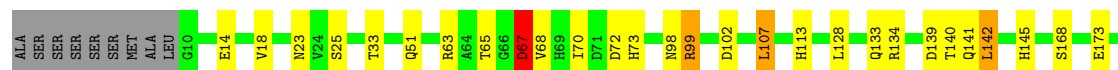
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain I:  71% 14% 12%

ALA SER SER SER SER MET ALA LEU G10 N29 T33 S40 D46 F58 D59 R63 A64 T65 G66 D67 H73 L81 N98 R99 A105 P106 L107 S119 Y123 L128 Q133 R134 V135 D139 T140 Q141 L142 H145 S149 L150 S154



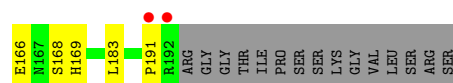
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

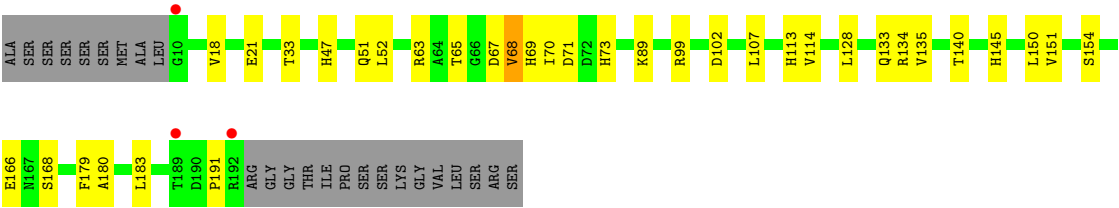


- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

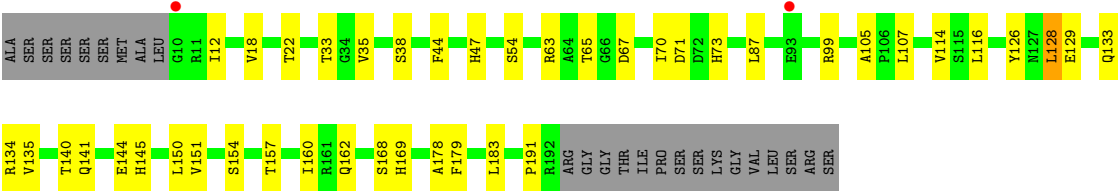


- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

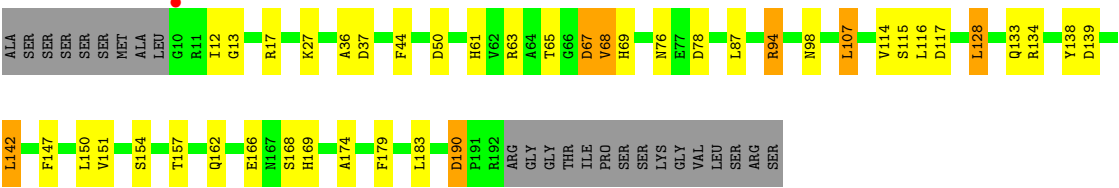




● Molecule 1: Imidazoglycerol-phosphate dehydratase 1



● Molecule 1: Imidazoglycerol-phosphate dehydratase 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	157.95Å 157.95Å 479.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.00) 98.0 (20.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.240 , 0.286 0.228 , 0.227	Depositor DCC
R_{free} test set	4414 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22288	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.80% 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: MN, SO4

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	0.74	1/1412 (0.1%)	0.95	2/1921 (0.1%)
1	B	0.66	0/1412	0.94	0/1921
1	C	0.74	0/1412	0.95	1/1921 (0.1%)
1	D	0.70	0/1412	0.97	0/1921
1	E	0.74	0/1412	0.97	0/1921
1	F	0.66	0/1412	0.94	0/1921
1	G	0.73	0/1412	0.99	0/1921
1	H	0.73	0/1412	0.97	0/1921
1	I	0.72	0/1412	0.94	1/1921 (0.1%)
1	J	0.66	0/1412	0.94	0/1921
1	K	0.72	0/1412	0.98	0/1921
1	L	0.69	0/1412	0.94	1/1921 (0.1%)
1	M	0.73	1/1412 (0.1%)	0.94	0/1921
1	N	0.68	0/1412	0.94	0/1921
1	O	0.74	1/1412 (0.1%)	0.97	1/1921 (0.1%)
1	P	0.70	0/1412	0.96	0/1921
All	All	0.71	3/22592 (0.0%)	0.95	6/30736 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	48	MET	SD-CE	-5.87	1.64	1.79
1	A	48	MET	SD-CE	-5.42	1.66	1.79
1	O	35	VAL	CA-CB	5.28	1.59	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	67	ASP	CB-CA-C	-6.83	102.75	111.22
1	O	22	THR	N-CA-C	5.67	116.85	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	ASP	CB-CA-C	-5.41	104.52	111.22
1	A	22	THR	N-CA-C	5.39	116.46	108.86
1	A	28	ILE	N-CA-C	5.07	115.34	107.28

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	1386	0	1330	14	0
1	B	1386	0	1330	17	0
1	C	1386	0	1330	14	0
1	D	1386	0	1330	11	0
1	E	1386	0	1330	16	0
1	F	1386	0	1330	16	0
1	G	1386	0	1330	13	0
1	H	1386	0	1330	14	0
1	I	1386	0	1330	17	0
1	J	1386	0	1330	14	0
1	K	1386	0	1330	14	0
1	L	1386	0	1330	13	0
1	M	1386	0	1330	16	0
1	N	1386	0	1330	14	0
1	O	1386	0	1330	19	0
1	P	1386	0	1330	21	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
2	I	2	0	0	0	0
2	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
All	All	22288	0	21280	217	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 5.

The worst 5 of 217 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:141:GLN:HE22	1:F:168:SER:H	1.25	0.84
1:K:141:GLN:HE22	1:N:168:SER:H	1.33	0.73
1:I:168:SER:H	1:J:141:GLN:HE22	1.35	0.72
1:M:141:GLN:HE22	1:P:168:SER:H	1.36	0.72
1:H:150:LEU:O	1:H:154:SER:HB3	1.91	0.70

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	181/207 (87%)	170 (94%)	10 (6%)	1 (1%)	21	56
1	B	181/207 (87%)	167 (92%)	14 (8%)	0	100	100
1	C	181/207 (87%)	170 (94%)	10 (6%)	1 (1%)	21	56
1	D	181/207 (87%)	167 (92%)	13 (7%)	1 (1%)	21	56
1	E	181/207 (87%)	168 (93%)	10 (6%)	3 (2%)	7	32
1	F	181/207 (87%)	168 (93%)	12 (7%)	1 (1%)	21	56
1	G	181/207 (87%)	168 (93%)	10 (6%)	3 (2%)	7	32
1	H	181/207 (87%)	164 (91%)	15 (8%)	2 (1%)	11	43
1	I	181/207 (87%)	169 (93%)	10 (6%)	2 (1%)	11	43
1	J	181/207 (87%)	166 (92%)	12 (7%)	3 (2%)	7	32
1	K	181/207 (87%)	168 (93%)	11 (6%)	2 (1%)	11	43
1	L	181/207 (87%)	168 (93%)	12 (7%)	1 (1%)	21	56
1	M	181/207 (87%)	169 (93%)	11 (6%)	1 (1%)	21	56
1	N	181/207 (87%)	167 (92%)	12 (7%)	2 (1%)	11	43
1	O	181/207 (87%)	163 (90%)	17 (9%)	1 (1%)	21	56
1	P	181/207 (87%)	167 (92%)	12 (7%)	2 (1%)	11	43
All	All	2896/3312 (87%)	2679 (92%)	191 (7%)	26 (1%)	14	48

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	67	ASP
1	N	68	VAL
1	E	67	ASP
1	G	67	ASP
1	P	68	VAL

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	145/171 (85%)	132 (91%)	13 (9%)	9	34
1	B	145/171 (85%)	131 (90%)	14 (10%)	8	30
1	C	145/171 (85%)	131 (90%)	14 (10%)	8	30
1	D	145/171 (85%)	134 (92%)	11 (8%)	12	41
1	E	145/171 (85%)	135 (93%)	10 (7%)	14	45
1	F	145/171 (85%)	131 (90%)	14 (10%)	8	30
1	G	145/171 (85%)	136 (94%)	9 (6%)	16	49
1	H	145/171 (85%)	133 (92%)	12 (8%)	10	37
1	I	145/171 (85%)	133 (92%)	12 (8%)	10	37
1	J	145/171 (85%)	133 (92%)	12 (8%)	10	37
1	K	145/171 (85%)	130 (90%)	15 (10%)	7	28
1	L	145/171 (85%)	128 (88%)	17 (12%)	5	23
1	M	145/171 (85%)	131 (90%)	14 (10%)	8	30
1	N	145/171 (85%)	131 (90%)	14 (10%)	8	30
1	O	145/171 (85%)	130 (90%)	15 (10%)	7	28
1	P	145/171 (85%)	132 (91%)	13 (9%)	9	34
All	All	2320/2736 (85%)	2111 (91%)	209 (9%)	9	34

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	107	LEU
1	L	116	LEU
1	P	67	ASP
1	J	142	LEU
1	K	140	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	162	GLN
1	P	61	HIS
1	G	127	ASN
1	G	76	ASN
1	P	73	HIS

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 48 ligands modelled in this entry, 32 are monoatomic - leaving 16 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	SO4	I	398	-	4,4,4	0.55	0	6,6,6	0.35	0
3	SO4	B	398	-	4,4,4	0.72	0	6,6,6	0.25	0
3	SO4	N	398	-	4,4,4	0.59	0	6,6,6	0.20	0
3	SO4	A	398	-	4,4,4	0.51	0	6,6,6	0.56	0
3	SO4	F	398	-	4,4,4	0.72	0	6,6,6	0.18	0
3	SO4	O	398	-	4,4,4	0.56	0	6,6,6	0.26	0
3	SO4	M	398	-	4,4,4	0.53	0	6,6,6	0.18	0
3	SO4	C	398	-	4,4,4	0.56	0	6,6,6	0.39	0
3	SO4	P	398	-	4,4,4	0.60	0	6,6,6	0.14	0
3	SO4	J	398	-	4,4,4	0.57	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	E	398	-	4,4,4	0.56	0	6,6,6	0.34	0
3	SO4	H	398	-	4,4,4	0.66	0	6,6,6	0.50	0
3	SO4	D	398	-	4,4,4	0.68	0	6,6,6	0.35	0
3	SO4	G	398	-	4,4,4	0.65	0	6,6,6	0.41	0
3	SO4	K	398	-	4,4,4	0.64	0	6,6,6	0.38	0
3	SO4	L	398	-	4,4,4	0.69	0	6,6,6	0.35	0

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 [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	183/207 (88%)	-0.07	0 100 100	17, 17, 17, 17	0
1	B	183/207 (88%)	-0.19	1 (0%) 87 72	17, 17, 17, 17	0
1	C	183/207 (88%)	-0.05	1 (0%) 87 72	17, 17, 17, 17	0
1	D	183/207 (88%)	-0.11	1 (0%) 87 72	17, 17, 17, 17	0
1	E	183/207 (88%)	-0.08	0 100 100	17, 17, 17, 17	0
1	F	183/207 (88%)	-0.16	2 (1%) 78 57	17, 17, 17, 17	0
1	G	183/207 (88%)	-0.06	0 100 100	17, 17, 17, 17	0
1	H	183/207 (88%)	-0.01	1 (0%) 87 72	17, 17, 17, 17	0
1	I	183/207 (88%)	-0.06	0 100 100	17, 17, 17, 17	0
1	J	183/207 (88%)	-0.14	1 (0%) 87 72	17, 17, 17, 17	0
1	K	183/207 (88%)	0.01	1 (0%) 87 72	17, 17, 17, 17	0
1	L	183/207 (88%)	-0.04	2 (1%) 78 57	17, 17, 17, 17	0
1	M	183/207 (88%)	-0.07	0 100 100	17, 17, 17, 17	0
1	N	183/207 (88%)	-0.10	3 (1%) 70 47	17, 17, 17, 17	0
1	O	183/207 (88%)	-0.00	2 (1%) 78 57	17, 17, 17, 17	0
1	P	183/207 (88%)	-0.07	1 (0%) 87 72	17, 17, 17, 17	0
All	All	2928/3312 (88%)	-0.08	16 (0%) 87 72	17, 17, 17, 17	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	10	GLY	3.5
1	K	25	SER	3.3
1	L	192	ARG	3.2
1	O	10	GLY	3.2
1	C	93	GLU	3.0

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
3	SO4	G	398	5/5	0.85	0.20	17,17,17,17	0
3	SO4	H	398	5/5	0.87	0.31	17,17,17,17	0
3	SO4	K	398	5/5	0.89	0.21	17,17,17,17	0
3	SO4	E	398	5/5	0.91	0.28	17,17,17,17	0
3	SO4	N	398	5/5	0.91	0.23	17,17,17,17	0
3	SO4	D	398	5/5	0.92	0.26	17,17,17,17	0
3	SO4	C	398	5/5	0.93	0.24	17,17,17,17	0
3	SO4	I	398	5/5	0.93	0.27	17,17,17,17	0
3	SO4	J	398	5/5	0.94	0.26	17,17,17,17	0
2	MN	D	300	1/1	0.94	0.07	17,17,17,17	0
3	SO4	A	398	5/5	0.94	0.26	17,17,17,17	0
2	MN	I	301	1/1	0.95	0.06	17,17,17,17	0
2	MN	C	300	1/1	0.95	0.10	17,17,17,17	0
3	SO4	B	398	5/5	0.95	0.21	17,17,17,17	0
3	SO4	L	398	5/5	0.95	0.24	17,17,17,17	0
2	MN	H	300	1/1	0.95	0.10	17,17,17,17	0
3	SO4	F	398	5/5	0.96	0.24	17,17,17,17	0
2	MN	M	300	1/1	0.96	0.06	17,17,17,17	0
2	MN	C	301	1/1	0.96	0.04	17,17,17,17	0
2	MN	G	300	1/1	0.96	0.07	17,17,17,17	0
3	SO4	O	398	5/5	0.96	0.23	17,17,17,17	0
2	MN	J	300	1/1	0.97	0.06	17,17,17,17	0
2	MN	K	300	1/1	0.97	0.06	17,17,17,17	0
2	MN	A	300	1/1	0.97	0.08	17,17,17,17	0
2	MN	P	300	1/1	0.97	0.09	17,17,17,17	0
3	SO4	M	398	5/5	0.97	0.18	17,17,17,17	0
2	MN	D	301	1/1	0.97	0.03	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	F	300	1/1	0.97	0.06	17,17,17,17	0
3	SO4	P	398	5/5	0.97	0.26	17,17,17,17	0
2	MN	O	301	1/1	0.98	0.04	17,17,17,17	0
2	MN	B	300	1/1	0.98	0.06	17,17,17,17	0
2	MN	E	300	1/1	0.98	0.08	17,17,17,17	0
2	MN	E	301	1/1	0.98	0.03	17,17,17,17	0
2	MN	L	300	1/1	0.98	0.06	17,17,17,17	0
2	MN	L	301	1/1	0.98	0.05	17,17,17,17	0
2	MN	I	300	1/1	0.98	0.08	17,17,17,17	0
2	MN	N	300	1/1	0.98	0.08	17,17,17,17	0
2	MN	O	300	1/1	0.98	0.07	17,17,17,17	0
2	MN	J	301	1/1	0.99	0.02	17,17,17,17	0
2	MN	A	301	1/1	0.99	0.09	17,17,17,17	0
2	MN	K	301	1/1	0.99	0.02	17,17,17,17	0
2	MN	P	301	1/1	0.99	0.04	17,17,17,17	0
2	MN	H	301	1/1	0.99	0.05	17,17,17,17	0
2	MN	F	301	1/1	0.99	0.02	17,17,17,17	0
2	MN	B	301	1/1	0.99	0.02	17,17,17,17	0
2	MN	M	301	1/1	0.99	0.03	17,17,17,17	0
2	MN	G	301	1/1	0.99	0.04	17,17,17,17	0
2	MN	N	301	1/1	0.99	0.07	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.