



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:39 am BST

PDB ID : 2F1D
Title : X-Ray Structure of imidazoleglycerol-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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

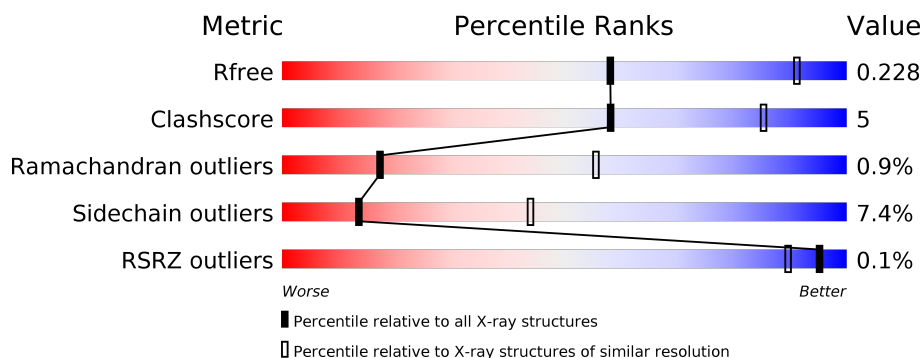
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	207	
1	B	207	
1	C	207	
1	D	207	
1	E	207	
1	F	207	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	207	 73%15%12%
1	H	207	 71%15%12%
1	I	207	 71%16%12%
1	J	207	 71%13%12%
1	K	207	 72%14%12%
1	L	207	 72%15%12%
1	M	207	 71%16%12%
1	N	207	 73%15%12%
1	O	207	 67%20%12%
1	P	207	 69%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 (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is SULFATE ION (three-letter code: 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		

Continued on next page...

Continued from previous page...

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 [i](#)

These plots are drawn for all protein, RNA and DNA 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.

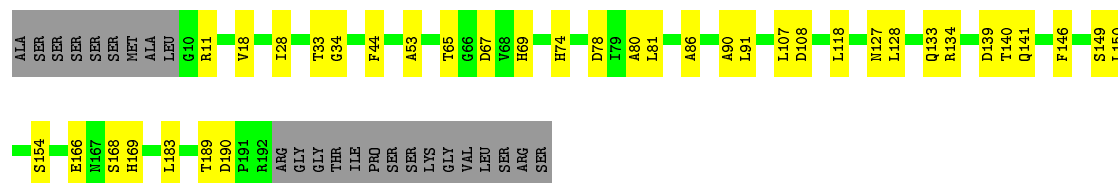
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain A: 



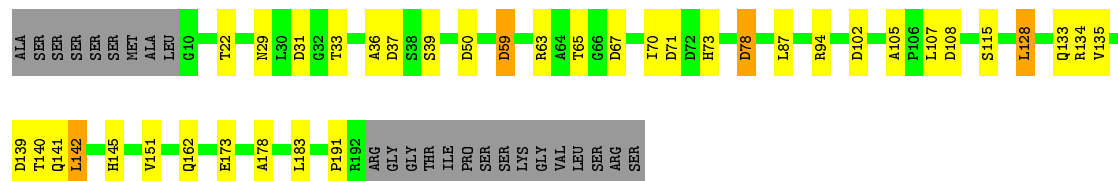
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain B: 




- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain C: 



- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain D: 



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

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain E:  71% 15% 12%

ALA
SER
SER
SER
SER
SER
SER
MET
ALA
LEU
G10
T33
D87
F44
H61
V62
R63
A64
T85
G66
D67
V68
H69
D72
D78
I79
A80
A105
P106
L107
D108
V114
D117
P122
L128
Q133
R134
V135
D139
T140
Q141
L142
F146
M156
Q162

H169
A174
A178
F179
L183
P191
R192
ARG
GLY
THR
ILE
PRO
SER
SER
LYS
GLY
VAL
LEU
SER
ARG
SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain F:  72% 14% 12%

ALA
SER
SER
SER
SER
SER
SER
MET
ALA
LEU
G10
V18
N23
D31
G32
T33
F44
H47
Q51
D59
R63
A64
G65
D67
H73
D78
R94
N98
D108
V114
M127
L128
Q133
R134
D139
T140
Q141
L142
H145
L150

S154
T160
S168
H169
F179
L183
D190
P191
R192
ARG
GLY
THR
ILE
PRO
SER
SER
LYS
GLY
VAL
LEU
SER
ARG
SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain G:  73% 15% 12%

ALA
SER
SER
SER
SER
SER
SER
MET
ALA
LEU
G10
L30
D31
G32
T33
A36
D37
H47
D50
D59
R63
D67
V68
H69
D72
H73
D78
L81
R99
D108
L116
D117
L118
Q133
R134
V135
D139
T140
Q141
L142
H145
S149
S168

L183
T187
R192
ARG
GLY
THR
ILE
PRO
SER
SER
LYS
GLY
VAL
LEU
SER
ARG
SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain H:  71% 15% 12%

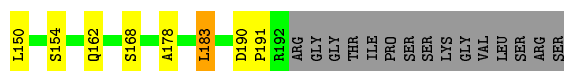
ALA
SER
SER
SER
SER
SER
SER
MET
ALA
LEU
G10
E21
S25
N29
T33
D37
F44
D59
V60
H61
R63
D67
V68
H69
I70
D78
D102
L107
D108
V114
S115
L116
L128
Q133
R134
D139
T140
Q141
L142
L150
S154
S168

H169
A174
F179
A180
R181
A182
L183
D190
P191
R192
ARG
GLY
THR
ILE
PRO
SER
SER
LYS
GLY
VAL
LEU
SER
ARG
SER

- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

Chain I:  71% 16% 12%

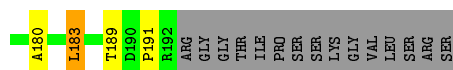
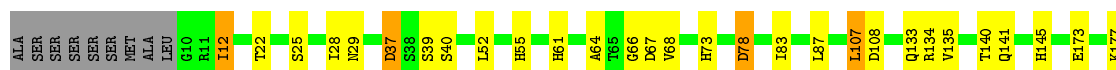
ALA
SER
SER
SER
SER
SER
SER
MET
ALA
LEU
G10
N29
T33
D37
S40
D46
F58
D59
R63
A64
T65
G66
D67
H73
L81
N98
R99
A105
P106
L107
D108
D117
Y123
L128
Q133
R134
V135
D139
T140
Q141
L142
H145
S149



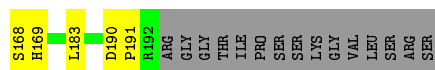
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



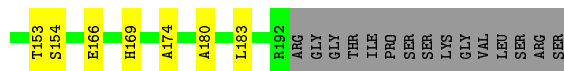
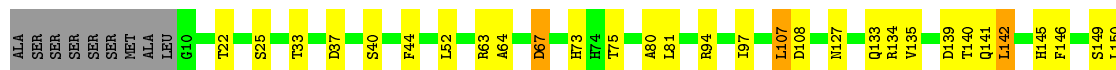
- Molecule 1: Imidazoglycerol-phosphate dehydratase 1



- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

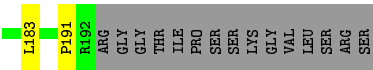


- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

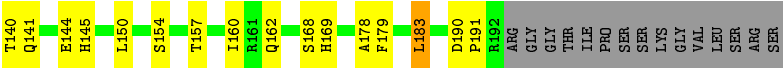


- Molecule 1: Imidazoglycerol-phosphate dehydratase 1

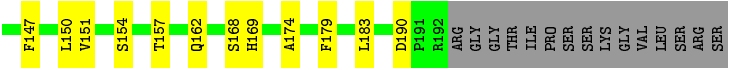
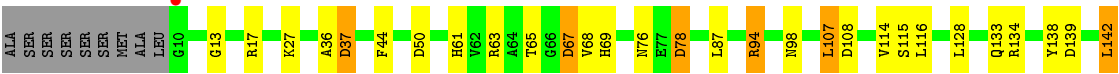




• Molecule 1: Imidazoglycerol-phosphate dehydratase 1



• 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) 98.3 (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 , 0.228	Depositor DCC
R_{free} test set	4414 reflections (5.04%)	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 , -0.3	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	0.50	0/1412	0.85	5/1921 (0.3%)
1	B	0.48	0/1412	0.82	3/1921 (0.2%)
1	C	0.52	0/1412	0.85	6/1921 (0.3%)
1	D	0.50	0/1412	0.83	3/1921 (0.2%)
1	E	0.52	0/1412	0.85	4/1921 (0.2%)
1	F	0.47	0/1412	0.84	5/1921 (0.3%)
1	G	0.50	0/1412	0.84	7/1921 (0.4%)
1	H	0.53	0/1412	0.85	4/1921 (0.2%)
1	I	0.51	0/1412	0.83	3/1921 (0.2%)
1	J	0.48	0/1412	0.84	9/1921 (0.5%)
1	K	0.51	0/1412	0.83	3/1921 (0.2%)
1	L	0.50	0/1412	0.82	5/1921 (0.3%)
1	M	0.50	0/1412	0.82	2/1921 (0.1%)
1	N	0.49	0/1412	0.83	2/1921 (0.1%)
1	O	0.53	0/1412	0.84	5/1921 (0.3%)
1	P	0.49	0/1412	0.82	3/1921 (0.2%)
All	All	0.50	0/22592	0.84	69/30736 (0.2%)

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ASP	CB-CG-OD2	7.66	125.19	118.30
1	O	108	ASP	CB-CG-OD2	7.59	125.13	118.30
1	B	108	ASP	CB-CG-OD2	7.57	125.11	118.30
1	I	108	ASP	CB-CG-OD2	7.48	125.03	118.30
1	E	78	ASP	CB-CG-OD2	7.32	124.89	118.30

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	13	0
1	B	1386	0	1330	15	0
1	C	1386	0	1330	14	0
1	D	1386	0	1330	10	0
1	E	1386	0	1330	14	0
1	F	1386	0	1330	15	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	15	0
1	K	1386	0	1330	14	0
1	L	1386	0	1330	13	0
1	M	1386	0	1330	15	0
1	N	1386	0	1330	14	0
1	O	1386	0	1330	19	0
1	P	1386	0	1330	19	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	208	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 208 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 [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	181/207 (87%)	170 (94%)	10 (6%)	1 (1%)	25 64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	181/207 (87%)	167 (92%)	14 (8%)	0	100	100
1	C	181/207 (87%)	170 (94%)	10 (6%)	1 (1%)	25	64
1	D	181/207 (87%)	167 (92%)	13 (7%)	1 (1%)	25	64
1	E	181/207 (87%)	168 (93%)	10 (6%)	3 (2%)	9	39
1	F	181/207 (87%)	168 (93%)	12 (7%)	1 (1%)	25	64
1	G	181/207 (87%)	168 (93%)	10 (6%)	3 (2%)	9	39
1	H	181/207 (87%)	164 (91%)	15 (8%)	2 (1%)	14	50
1	I	181/207 (87%)	169 (93%)	10 (6%)	2 (1%)	14	50
1	J	181/207 (87%)	166 (92%)	12 (7%)	3 (2%)	9	39
1	K	181/207 (87%)	168 (93%)	11 (6%)	2 (1%)	14	50
1	L	181/207 (87%)	168 (93%)	12 (7%)	1 (1%)	25	64
1	M	181/207 (87%)	169 (93%)	11 (6%)	1 (1%)	25	64
1	N	181/207 (87%)	167 (92%)	12 (7%)	2 (1%)	14	50
1	O	181/207 (87%)	163 (90%)	17 (9%)	1 (1%)	25	64
1	P	181/207 (87%)	167 (92%)	12 (7%)	2 (1%)	14	50
All	All	2896/3312 (87%)	2679 (92%)	191 (7%)	26 (1%)	17	55

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%)	133 (92%)	12 (8%)	11	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	145/171 (85%)	134 (92%)	11 (8%)	13	43
1	C	145/171 (85%)	131 (90%)	14 (10%)	8	31
1	D	145/171 (85%)	135 (93%)	10 (7%)	15	48
1	E	145/171 (85%)	136 (94%)	9 (6%)	18	52
1	F	145/171 (85%)	133 (92%)	12 (8%)	11	39
1	G	145/171 (85%)	138 (95%)	7 (5%)	25	62
1	H	145/171 (85%)	134 (92%)	11 (8%)	13	43
1	I	145/171 (85%)	137 (94%)	8 (6%)	21	57
1	J	145/171 (85%)	135 (93%)	10 (7%)	15	48
1	K	145/171 (85%)	136 (94%)	9 (6%)	18	52
1	L	145/171 (85%)	132 (91%)	13 (9%)	9	35
1	M	145/171 (85%)	133 (92%)	12 (8%)	11	39
1	N	145/171 (85%)	136 (94%)	9 (6%)	18	52
1	O	145/171 (85%)	130 (90%)	15 (10%)	7	28
1	P	145/171 (85%)	136 (94%)	9 (6%)	18	52
All	All	2320/2736 (85%)	2149 (93%)	171 (7%)	13	44

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	63	ARG
1	J	33	THR
1	O	134	ARG
1	H	128	LEU
1	I	33	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	133	GLN
1	J	61	HIS
1	P	61	HIS
1	H	162	GLN
1	I	133	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	J	398	-	4,4,4	0.48	0	6,6,6	0.31	0
3	SO4	I	398	-	4,4,4	0.47	0	6,6,6	0.37	0
3	SO4	L	398	-	4,4,4	0.62	0	6,6,6	0.40	0
3	SO4	N	398	-	4,4,4	0.50	0	6,6,6	0.21	0
3	SO4	M	398	-	4,4,4	0.44	0	6,6,6	0.20	0
3	SO4	G	398	-	4,4,4	0.58	0	6,6,6	0.41	0
3	SO4	B	398	-	4,4,4	0.65	0	6,6,6	0.30	0
3	SO4	A	398	-	4,4,4	0.42	0	6,6,6	0.57	0
3	SO4	D	398	-	4,4,4	0.60	0	6,6,6	0.36	0
3	SO4	K	398	-	4,4,4	0.57	0	6,6,6	0.36	0
3	SO4	F	398	-	4,4,4	0.64	0	6,6,6	0.18	0
3	SO4	E	398	-	4,4,4	0.48	0	6,6,6	0.33	0
3	SO4	C	398	-	4,4,4	0.47	0	6,6,6	0.36	0
3	SO4	P	398	-	4,4,4	0.51	0	6,6,6	0.11	0
3	SO4	H	398	-	4,4,4	0.58	0	6,6,6	0.48	0
3	SO4	O	398	-	4,4,4	0.47	0	6,6,6	0.31	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%)	-0.67	0	100	100	17, 17, 17, 17	0
1	B	183/207 (88%)	-0.67	0	100	100	17, 17, 17, 17	0
1	C	183/207 (88%)	-0.59	0	100	100	17, 17, 17, 17	0
1	D	183/207 (88%)	-0.64	0	100	100	17, 17, 17, 17	0
1	E	183/207 (88%)	-0.60	0	100	100	17, 17, 17, 17	0
1	F	183/207 (88%)	-0.70	0	100	100	17, 17, 17, 17	0
1	G	183/207 (88%)	-0.59	0	100	100	17, 17, 17, 17	0
1	H	183/207 (88%)	-0.60	0	100	100	17, 17, 17, 17	0
1	I	183/207 (88%)	-0.64	0	100	100	17, 17, 17, 17	0
1	J	183/207 (88%)	-0.68	0	100	100	17, 17, 17, 17	0
1	K	183/207 (88%)	-0.60	0	100	100	17, 17, 17, 17	0
1	L	183/207 (88%)	-0.63	0	100	100	17, 17, 17, 17	0
1	M	183/207 (88%)	-0.63	0	100	100	17, 17, 17, 17	0
1	N	183/207 (88%)	-0.66	0	100	100	17, 17, 17, 17	0
1	O	183/207 (88%)	-0.56	1 (0%)	91	75	17, 17, 17, 17	0
1	P	183/207 (88%)	-0.62	1 (0%)	91	75	17, 17, 17, 17	0
All	All	2928/3312 (88%)	-0.63	2 (0%)	95	89	17, 17, 17, 17	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	10	GLY	2.3
1	P	10	GLY	2.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	SO4	H	398	5/5	0.90	0.44	17,17,17,17	0
3	SO4	B	398	5/5	0.91	0.35	17,17,17,17	0
3	SO4	E	398	5/5	0.91	0.38	17,17,17,17	0
2	MN	C	301	1/1	0.92	0.06	17,17,17,17	0
3	SO4	N	398	5/5	0.92	0.33	17,17,17,17	0
3	SO4	K	398	5/5	0.93	0.30	17,17,17,17	0
3	SO4	G	398	5/5	0.93	0.27	17,17,17,17	0
2	MN	C	300	1/1	0.94	0.14	17,17,17,17	0
2	MN	D	300	1/1	0.94	0.10	17,17,17,17	0
3	SO4	I	398	5/5	0.95	0.39	17,17,17,17	0
2	MN	E	300	1/1	0.95	0.11	17,17,17,17	0
3	SO4	P	398	5/5	0.95	0.39	17,17,17,17	0
2	MN	P	300	1/1	0.95	0.10	17,17,17,17	0
3	SO4	L	398	5/5	0.95	0.36	17,17,17,17	0
3	SO4	O	398	5/5	0.95	0.34	17,17,17,17	0
3	SO4	C	398	5/5	0.95	0.33	17,17,17,17	0
3	SO4	F	398	5/5	0.95	0.38	17,17,17,17	0
3	SO4	D	398	5/5	0.96	0.41	17,17,17,17	0
2	MN	E	301	1/1	0.96	0.06	17,17,17,17	0
2	MN	I	301	1/1	0.96	0.08	17,17,17,17	0
3	SO4	A	398	5/5	0.96	0.37	17,17,17,17	0
2	MN	O	301	1/1	0.96	0.06	17,17,17,17	0
2	MN	D	301	1/1	0.97	0.04	17,17,17,17	0
2	MN	F	300	1/1	0.97	0.10	17,17,17,17	0
2	MN	G	300	1/1	0.97	0.06	17,17,17,17	0
2	MN	B	300	1/1	0.97	0.09	17,17,17,17	0
2	MN	O	300	1/1	0.97	0.12	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	H	300	1/1	0.97	0.09	17,17,17,17	0
2	MN	L	300	1/1	0.97	0.07	17,17,17,17	0
2	MN	F	301	1/1	0.97	0.03	17,17,17,17	0
2	MN	P	301	1/1	0.97	0.06	17,17,17,17	0
2	MN	M	300	1/1	0.97	0.09	17,17,17,17	0
3	SO4	J	398	5/5	0.97	0.36	17,17,17,17	0
2	MN	I	300	1/1	0.98	0.10	17,17,17,17	0
2	MN	L	301	1/1	0.98	0.10	17,17,17,17	0
2	MN	K	301	1/1	0.98	0.04	17,17,17,17	0
2	MN	M	301	1/1	0.98	0.04	17,17,17,17	0
2	MN	B	301	1/1	0.98	0.04	17,17,17,17	0
3	SO4	M	398	5/5	0.98	0.28	17,17,17,17	0
2	MN	J	300	1/1	0.98	0.09	17,17,17,17	0
2	MN	K	300	1/1	0.98	0.12	17,17,17,17	0
2	MN	A	300	1/1	0.98	0.11	17,17,17,17	0
2	MN	H	301	1/1	0.98	0.07	17,17,17,17	0
2	MN	A	301	1/1	0.99	0.12	17,17,17,17	0
2	MN	N	300	1/1	0.99	0.13	17,17,17,17	0
2	MN	G	301	1/1	0.99	0.03	17,17,17,17	0
2	MN	N	301	1/1	0.99	0.10	17,17,17,17	0
2	MN	J	301	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers

There are no such residues in this entry.