



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2024 – 08:59 AM JST

PDB ID : 6K31  
Title : Crystal structure of pyrophosphate-dependent phosphoenolpyruvate carboxykinase (PPi-PEPCK)  
Authors : Chiba, Y.; Miyakawa, T.; Tanokura, M.  
Deposited on : 2019-05-15  
Resolution : 2.60 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](mailto: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>.

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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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

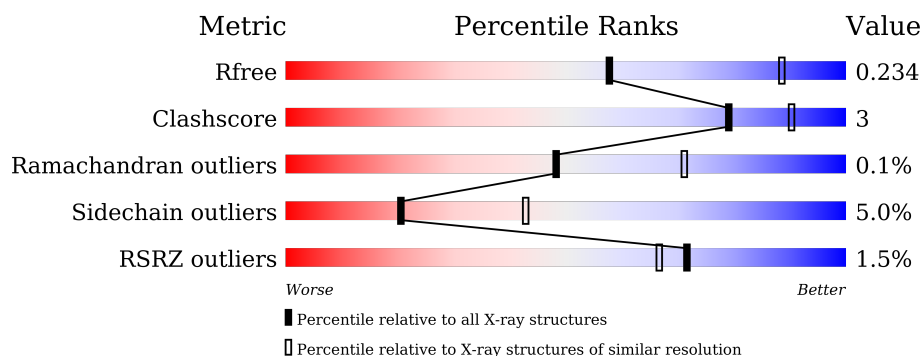
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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	1153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>7% . .</span> </div> </div>
1	B	1153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 86%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>86%</span> <span>8% . .</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17477 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 AiPEPCK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1109	Total	C	N	O	S	Se	0	0	0
			8568	5401	1519	1624	8	16			
1	B	1108	Total	C	N	O	S	Se	0	0	0
			8552	5391	1517	1620	8	16			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		

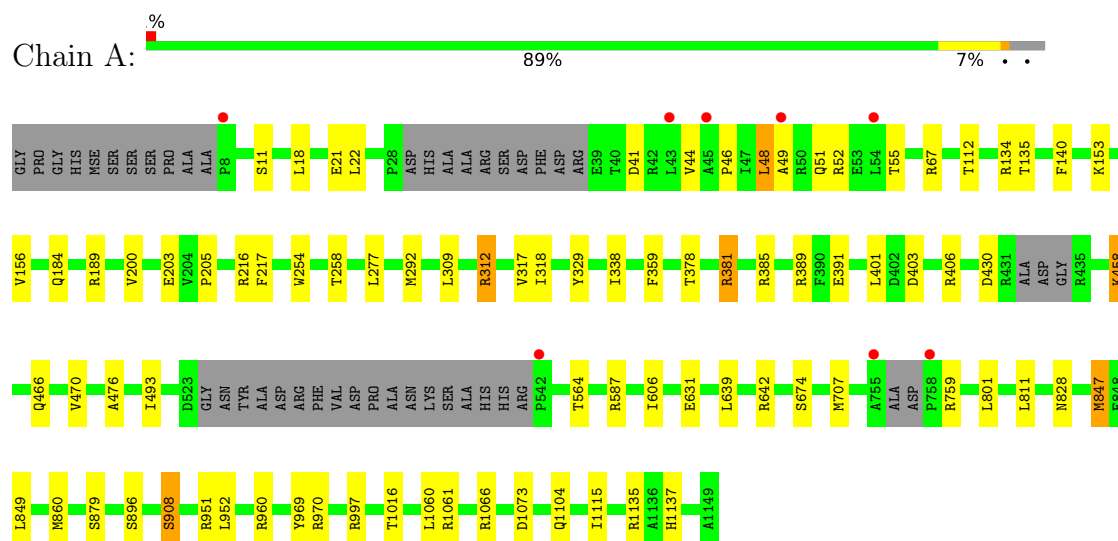
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total	O	0	0
			216	216		
3	B	139	Total	O	0	0
			139	139		

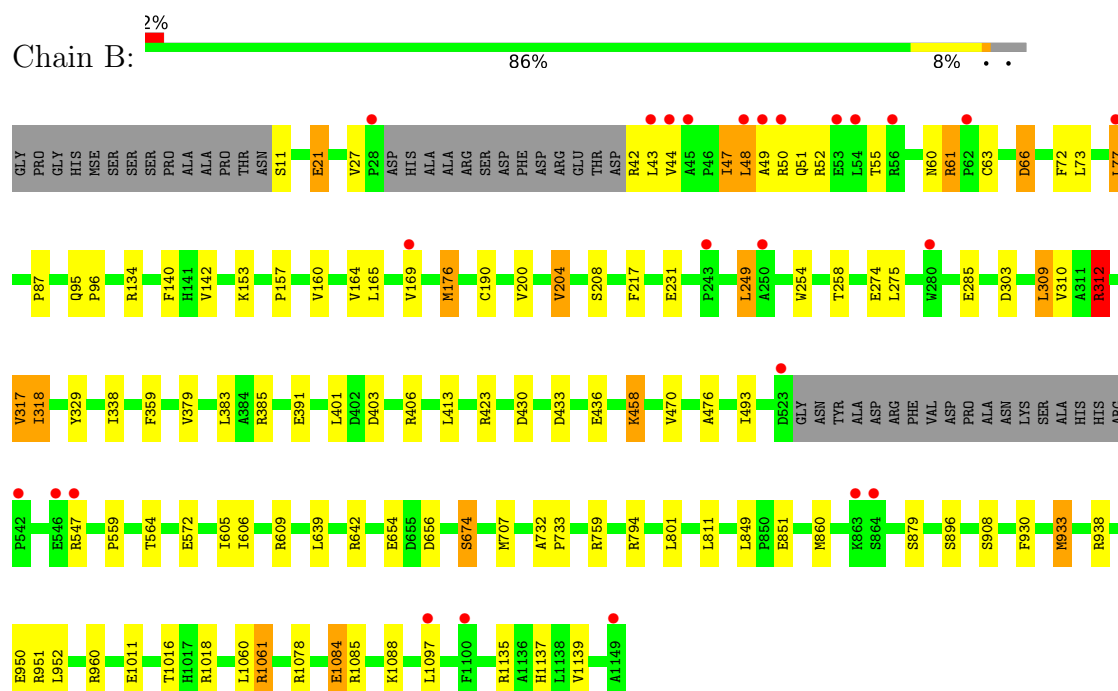
### 3 Residue-property plots

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: AiPEPCK



#### • Molecule 1: AiPEPCK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.44Å 160.44Å 200.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.12 – 2.60 48.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.12-2.60) 99.9 (48.12-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.60 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.196 , 0.241 0.195 , 0.234	Depositor DCC
$R_{free}$ test set	4627 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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:  
CO

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	0/8750	0.92	14/11879 (0.1%)
1	B	0.69	0/8735	0.90	9/11862 (0.1%)
All	All	0.72	0/17485	0.91	23/23741 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	A	312	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	A	312	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	933	MSE	CG-SE-CE	8.40	117.38	98.90
1	A	847	MSE	CG-SE-CE	-8.34	80.56	98.90
1	B	312	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	B	66	ASP	CB-CG-OD2	8.11	125.60	118.30
1	A	1066	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	B	707	MSE	CA-CB-CG	-7.64	100.30	113.30
1	A	707	MSE	CA-CB-CG	-7.17	101.10	113.30
1	A	189	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	1066	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	189	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	216	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	1061	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	1073	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	423	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	67	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	B	642	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	960	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	216	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	951	ARG	NE-CZ-NH1	5.10	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	656	ASP	CB-CG-OD1	5.02	122.82	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	8568	0	8433	27	0
1	B	8552	0	8417	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	216	0	0	1	0
3	B	139	0	0	5	0
All	All	17477	0	16850	88	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 3.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD21	1:B:165:LEU:HD21	1.61	0.83
1:B:860:MSE:HG3	1:B:1016:THR:HG21	1.72	0.71
1:A:860:MSE:HG3	1:A:1016:THR:HG21	1.72	0.71
1:A:18:LEU:C	1:A:18:LEU:HD23	2.11	0.71
1:B:933:MSE:HE3	1:B:938:ARG:CB	2.25	0.67
1:B:310:VAL:CG1	1:B:318:ILE:HD11	2.26	0.66
1:B:176:MSE:CE	1:B:190:CYS:O	2.45	0.64
1:B:204:VAL:HG23	1:B:208:SER:OG	1.99	0.63
1:B:960:ARG:NH1	1:B:1011:GLU:OE1	2.33	0.62
1:A:951:ARG:HD3	1:A:969:TYR:CZ	2.35	0.61
1:B:310:VAL:HG13	1:B:318:ILE:HD11	1.81	0.61
1:B:933:MSE:HE3	1:B:938:ARG:HB2	1.83	0.60
1:B:176:MSE:HE1	1:B:190:CYS:C	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:930:PHE:CD1	1:B:933:MSE:HE2	2.37	0.59
1:B:51:GLN:O	1:B:55:THR:HG23	2.03	0.58
1:A:51:GLN:O	1:A:55:THR:HG23	2.02	0.58
1:B:164:VAL:HG21	1:B:309:LEU:CD1	2.33	0.57
1:B:609:ARG:NH2	3:B:1306:HOH:O	2.37	0.56
1:B:21:GLU:HB3	1:B:48:LEU:HD11	1.87	0.56
1:B:933:MSE:HE3	1:B:938:ARG:HB3	1.88	0.56
1:B:63:CYS:SG	1:B:66:ASP:OD1	2.58	0.55
1:B:72:PHE:CG	1:B:317:VAL:HG22	2.43	0.54
1:B:61:ARG:O	1:B:61:ARG:HD2	2.08	0.53
1:B:458:LYS:HD3	1:B:470:VAL:HG21	1.90	0.53
1:A:458:LYS:HD3	1:A:470:VAL:HG21	1.90	0.53
1:B:1078:ARG:NH2	3:B:1303:HOH:O	2.32	0.52
1:B:157:PRO:HD2	1:B:160:VAL:HG11	1.91	0.52
1:A:153:LYS:NZ	1:A:879:SER:O	2.37	0.51
1:B:801:LEU:HD12	1:B:811:LEU:HD21	1.92	0.51
1:B:606:ILE:HD12	1:B:606:ILE:N	2.26	0.51
1:B:176:MSE:CE	1:B:190:CYS:C	2.78	0.51
1:B:44:VAL:O	1:B:44:VAL:HG12	2.11	0.51
1:A:134:ARG:HG3	1:A:329:TYR:CE1	2.47	0.50
1:A:277:LEU:HD21	1:A:292:MSE:HE3	1.94	0.50
1:B:164:VAL:HG21	1:B:309:LEU:HD12	1.93	0.50
1:A:801:LEU:HD12	1:A:811:LEU:HD21	1.95	0.49
1:B:930:PHE:HA	1:B:933:MSE:HE2	1.95	0.49
1:A:156:VAL:HA	1:A:292:MSE:HE2	1.94	0.49
1:B:96:PRO:HA	1:B:231:GLU:OE2	2.13	0.48
1:B:258:THR:O	1:B:317:VAL:HA	2.12	0.48
1:B:310:VAL:CG1	1:B:318:ILE:CD1	2.91	0.48
1:A:606:ILE:HD12	1:A:606:ILE:N	2.28	0.47
1:B:930:PHE:CD1	1:B:933:MSE:CE	2.97	0.47
1:A:378:THR:HG23	1:A:381:ARG:H	1.78	0.47
1:A:258:THR:O	1:A:317:VAL:HA	2.14	0.47
1:B:87:PRO:HD3	1:B:169:VAL:HG13	1.97	0.46
1:A:970:ARG:NH2	1:A:997:ARG:HD2	2.30	0.46
1:A:277:LEU:HD21	1:A:292:MSE:CE	2.46	0.46
1:B:160:VAL:HG23	1:B:275:LEU:HB3	1.96	0.46
1:A:18:LEU:HD23	1:A:22:LEU:HD12	1.98	0.46
1:B:134:ARG:HG3	1:B:329:TYR:CE1	2.51	0.46
1:B:153:LYS:NZ	1:B:879:SER:O	2.38	0.46
1:B:379:VAL:O	1:B:383:LEU:HD13	2.16	0.45
1:A:48:LEU:HD23	1:A:49:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:CE2	1:A:476:ALA:HB2	2.52	0.45
1:B:48:LEU:HD23	1:B:49:ALA:N	2.32	0.44
1:B:176:MSE:HE1	1:B:190:CYS:O	2.14	0.44
1:B:27:VAL:HG11	1:B:42:ARG:HH12	1.83	0.44
1:B:47:ILE:HA	1:B:50:ARG:HG3	2.00	0.44
1:B:200:VAL:HG22	1:B:338:ILE:HG23	1.99	0.44
1:B:249:LEU:HD12	1:B:1097:LEU:HD23	1.99	0.44
1:A:18:LEU:HD23	1:A:18:LEU:O	2.17	0.43
1:A:200:VAL:HG22	1:A:338:ILE:HG23	2.01	0.43
1:A:292:MSE:HE3	1:A:292:MSE:HB3	1.83	0.43
1:A:277:LEU:CD2	1:A:292:MSE:HE3	2.48	0.43
1:B:72:PHE:CG	1:B:317:VAL:CG2	3.02	0.43
1:B:47:ILE:H	1:B:47:ILE:HG13	1.48	0.43
1:B:605:ILE:HD12	1:B:605:ILE:N	2.34	0.42
1:B:157:PRO:HD2	1:B:160:VAL:CG1	2.49	0.42
1:B:1084:GLU:OE1	1:B:1088:LYS:HE3	2.20	0.42
1:A:391:GLU:HB2	1:A:401:LEU:HD21	2.02	0.42
1:B:732:ALA:N	1:B:733:PRO:CD	2.83	0.42
1:B:72:PHE:CD2	1:B:317:VAL:CG2	3.02	0.42
1:B:359:PHE:CE2	1:B:476:ALA:HB2	2.55	0.42
1:B:654:GLU:OE2	3:B:1302:HOH:O	2.22	0.42
1:A:828:ASN:ND2	1:A:908:SER:OG	2.53	0.42
1:B:142:VAL:CG1	1:B:312:ARG:NH1	2.83	0.42
1:B:559:PRO:HG3	1:B:572:GLU:OE2	2.20	0.42
1:A:18:LEU:C	1:A:18:LEU:CD2	2.85	0.41
1:B:391:GLU:HB2	1:B:401:LEU:HD21	2.02	0.41
1:B:851:GLU:OE2	1:B:1061:ARG:NH2	2.50	0.41
1:A:466:GLN:NE2	3:A:1333:HOH:O	2.53	0.41
1:B:176:MSE:HE3	1:B:176:MSE:HA	2.02	0.41
1:B:674:SER:O	3:B:1301:HOH:O	2.22	0.41
1:B:1085:ARG:HG2	3:B:1384:HOH:O	2.21	0.41
1:A:21:GLU:HB3	1:A:48:LEU:HD11	2.03	0.40
1:B:73:LEU:HD21	1:B:165:LEU:CD2	2.43	0.40
1:B:77:LEU:N	1:B:77:LEU:HD23	2.36	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	1099/1153 (95%)	1054 (96%)	44 (4%)	1 (0%)	48	71
1	B	1102/1153 (96%)	1052 (96%)	49 (4%)	1 (0%)	48	71
All	All	2201/2306 (95%)	2106 (96%)	93 (4%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	436	GLU
1	A	46	PRO

### 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	895/909 (98%)	854 (95%)	41 (5%)	23	46
1	B	891/909 (98%)	842 (94%)	49 (6%)	18	38
All	All	1786/1818 (98%)	1696 (95%)	90 (5%)	20	43

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	41	ASP
1	A	44	VAL
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	52	ARG
1	A	112	THR
1	A	135	THR
1	A	140	PHE
1	A	184	GLN
1	A	203	GLU
1	A	205	PRO
1	A	217	PHE
1	A	254	TRP
1	A	309	LEU
1	A	312	ARG
1	A	318	ILE
1	A	381	ARG
1	A	385	ARG
1	A	389	ARG
1	A	403	ASP
1	A	406	ARG
1	A	430	ASP
1	A	458	LYS
1	A	493	ILE
1	A	564	THR
1	A	587	ARG
1	A	631	GLU
1	A	639	LEU
1	A	642	ARG
1	A	674	SER
1	A	759	ARG
1	A	847	MSE
1	A	849	LEU
1	A	896	SER
1	A	908	SER
1	A	952	LEU
1	A	1060	LEU
1	A	1104	GLN
1	A	1115	ILE
1	A	1135	ARG
1	A	1137	HIS
1	B	11	SER
1	B	21	GLU
1	B	43	LEU
1	B	47	ILE
1	B	48	LEU

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Mol	Chain	Res	Type
1	B	52	ARG
1	B	60	ASN
1	B	61	ARG
1	B	77	LEU
1	B	95	GLN
1	B	140	PHE
1	B	176	MSE
1	B	204	VAL
1	B	217	PHE
1	B	249	LEU
1	B	254	TRP
1	B	274	GLU
1	B	285	GLU
1	B	303	ASP
1	B	309	LEU
1	B	312	ARG
1	B	317	VAL
1	B	318	ILE
1	B	385	ARG
1	B	403	ASP
1	B	406	ARG
1	B	413	LEU
1	B	430	ASP
1	B	433	ASP
1	B	458	LYS
1	B	493	ILE
1	B	547	ARG
1	B	564	THR
1	B	639	LEU
1	B	674	SER
1	B	759	ARG
1	B	794	ARG
1	B	849	LEU
1	B	896	SER
1	B	908	SER
1	B	950	GLU
1	B	952	LEU
1	B	1018	ARG
1	B	1060	LEU
1	B	1061	ARG
1	B	1084	GLU
1	B	1135	ARG

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Mol	Chain	Res	Type
1	B	1137	HIS
1	B	1139	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	792	ASN
1	A	828	ASN
1	A	1137	HIS
1	B	257	HIS
1	B	302	ASN

### 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 2 ligands modelled in this entry, 2 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1093/1153 (94%)	-0.45	8 (0%) 84 81	26, 44, 82, 133	0
1	B	1092/1153 (94%)	0.05	25 (2%) 61 55	30, 57, 99, 152	0
All	All	2185/2306 (94%)	-0.20	33 (1%) 71 67	26, 50, 91, 152	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	PRO	4.4
1	B	50	ARG	4.0
1	B	547	ARG	3.9
1	B	43	LEU	3.7
1	A	758	PRO	3.6
1	B	1149	ALA	3.3
1	B	54	LEU	3.2
1	A	542	PRO	3.2
1	B	1100	PHE	3.0
1	A	8	PRO	2.9
1	A	755	ALA	2.9
1	B	28	PRO	2.9
1	A	54	LEU	2.7
1	B	53	GLU	2.7
1	A	43	LEU	2.7
1	B	48	LEU	2.7
1	B	523	ASP	2.6
1	B	62	PRO	2.6
1	B	49	ALA	2.6
1	A	45	ALA	2.5
1	B	44	VAL	2.4
1	B	45	ALA	2.4
1	B	1097	LEU	2.3
1	B	56	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	250	ALA	2.2
1	B	864	SER	2.2
1	B	77	LEU	2.2
1	B	280	TRP	2.2
1	B	243	PRO	2.1
1	B	546	GLU	2.1
1	A	49	ALA	2.1
1	B	863	LYS	2.1
1	B	169	VAL	2.1

## 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 monosaccharides 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, 95<sup>th</sup> 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.

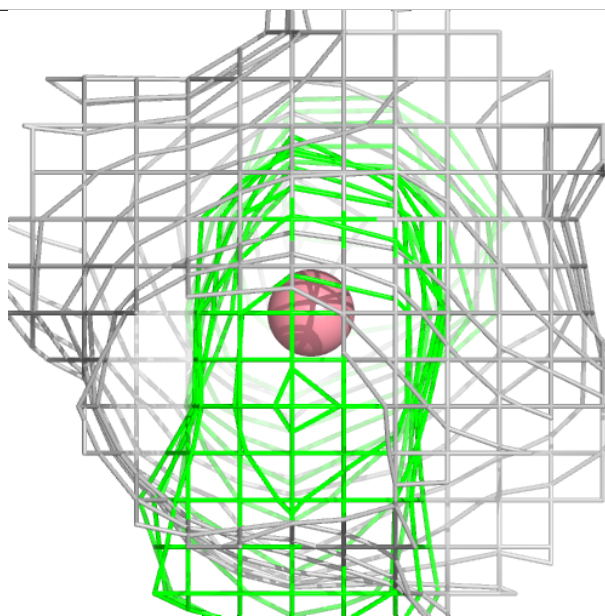
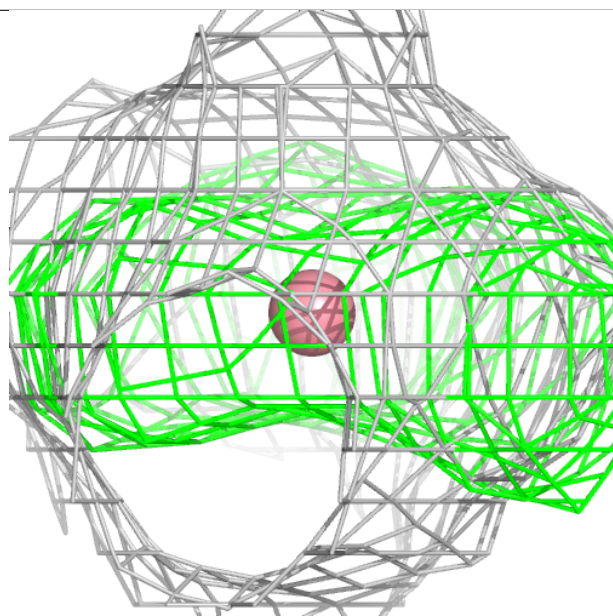
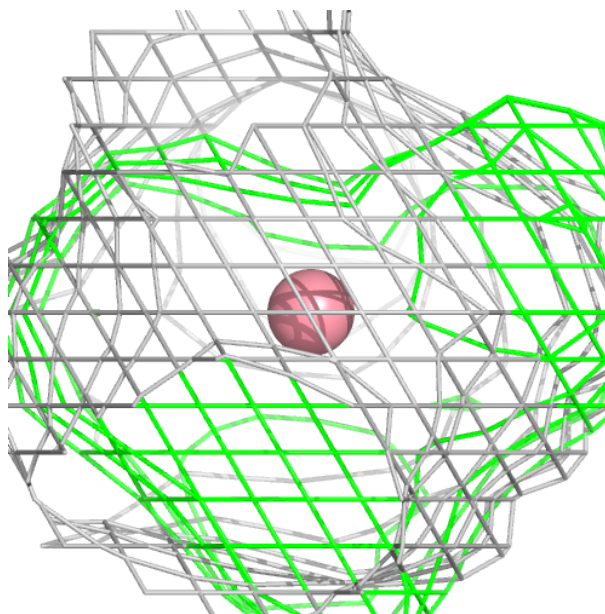
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO	A	1201	1/1	0.98	0.09	37,37,37,37	0
2	CO	B	1201	1/1	0.98	0.10	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



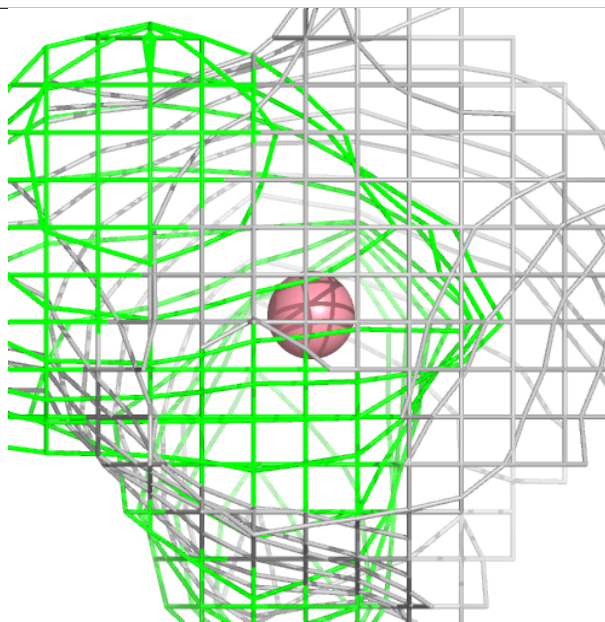
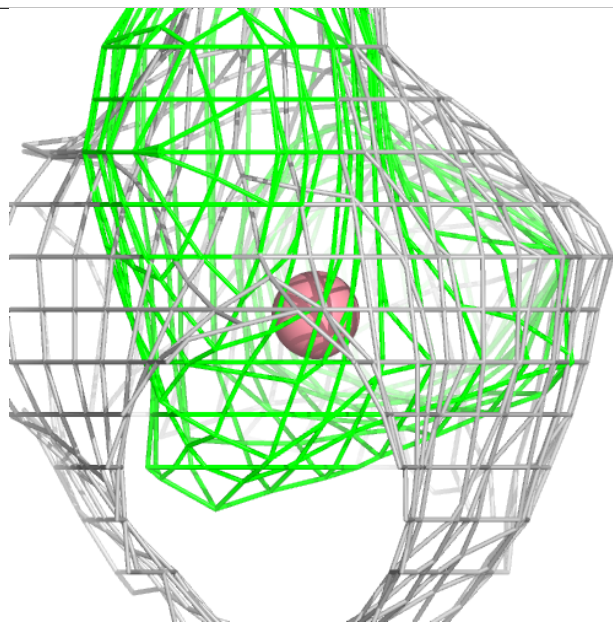
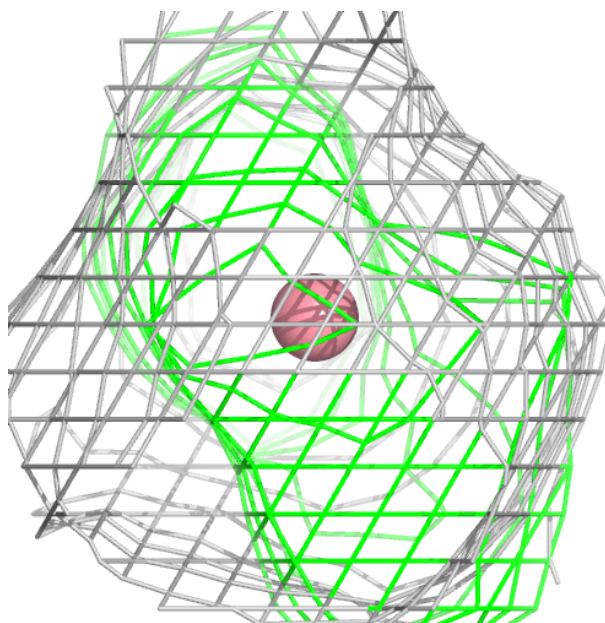
**Electron density around CO A 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CO B 1201:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.