



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 07:39 PM EST

PDB ID : 1JXZ  
Title : Structure of the H90Q mutant of 4-Chlorobenzoyl-Coenzyme A Dehalogenase complexed with 4-hydroxybenzoyl-Coenzyme A (product)  
Authors : Thoden, J.B.; Zhang, W.; Wei, Y.; Luo, L.; Taylor, K.L.; Yang, G.; Dunaway-Mariano, D.; Benning, M.M.; Holden, H.M.  
Deposited on : 2001-09-10  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

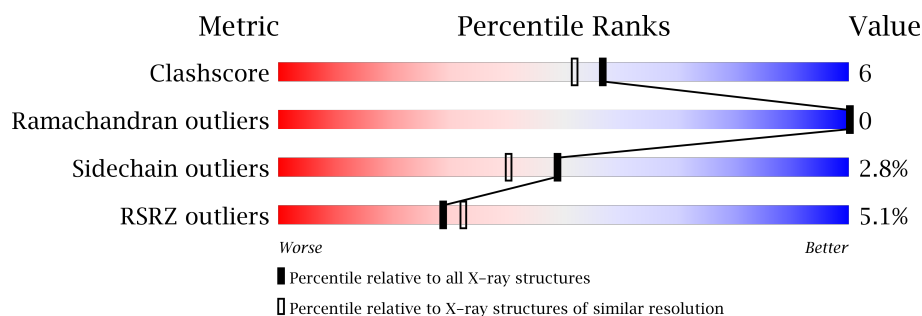
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	269	 78% 22%
1	B	269	 4% 75% 21% ..
1	C	269	 10% 72% 22% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	B	271	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7199 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 4-chlorobenzoyl Coenzyme A dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	1	0
			2088	1319	377	377	15			
1	B	269	Total	C	N	O	S	0	2	0
			2097	1324	378	379	16			
1	C	264	Total	C	N	O	S	0	1	0
			2051	1299	365	371	16			

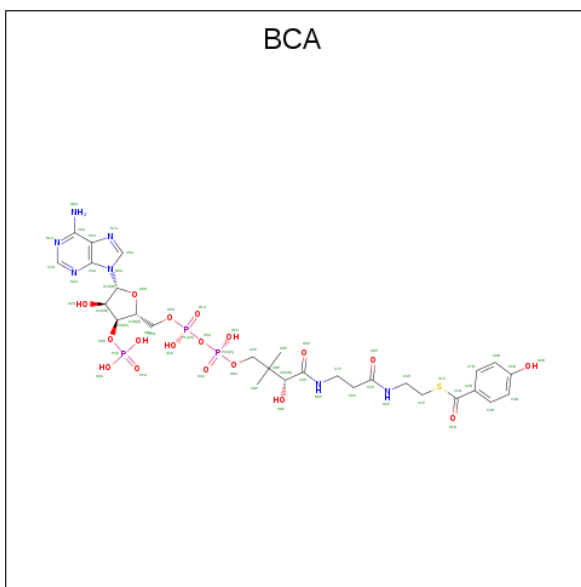
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	GLY	CONFLICT	PIR 419529
A	90	GLN	HIS	ENGINEERED	PIR 419529
B	85	ALA	GLY	CONFLICT	PIR 419529
B	90	GLN	HIS	ENGINEERED	PIR 419529
C	85	ALA	GLY	CONFLICT	PIR 419529
C	90	GLN	HIS	ENGINEERED	PIR 419529

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

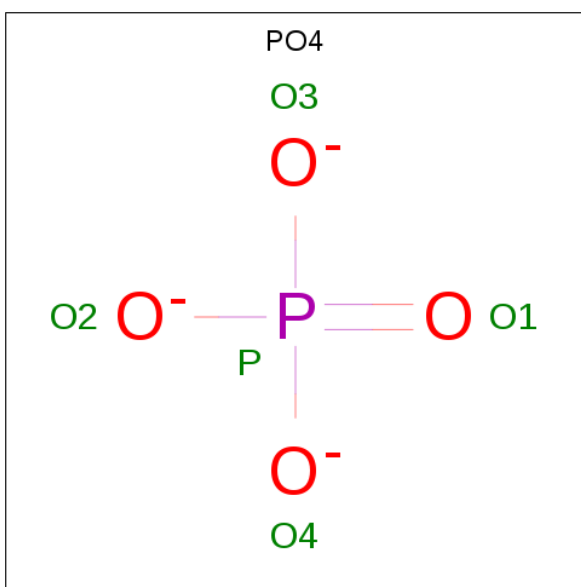
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 4-HYDROXYBENZOYL COENZYME A (three-letter code: BCA) (formula: C<sub>28</sub>H<sub>40</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			53	28	7	15	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			53	28	7	15	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			53	28	7	15	2	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

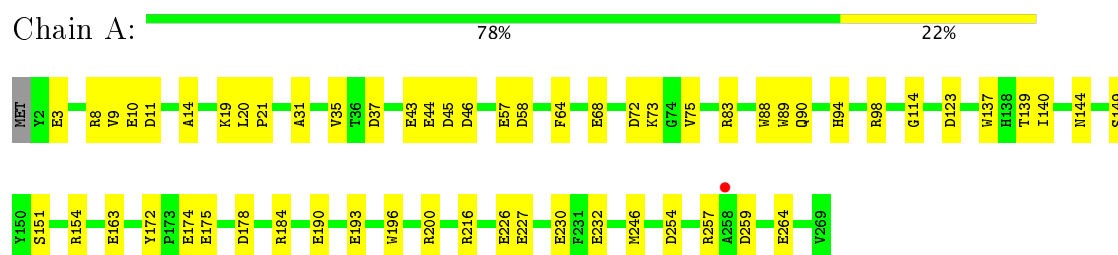
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	324	Total 324	O 324	0	0
5	B	248	Total 248	O 248	0	0
5	C	224	Total 224	O 224	0	0

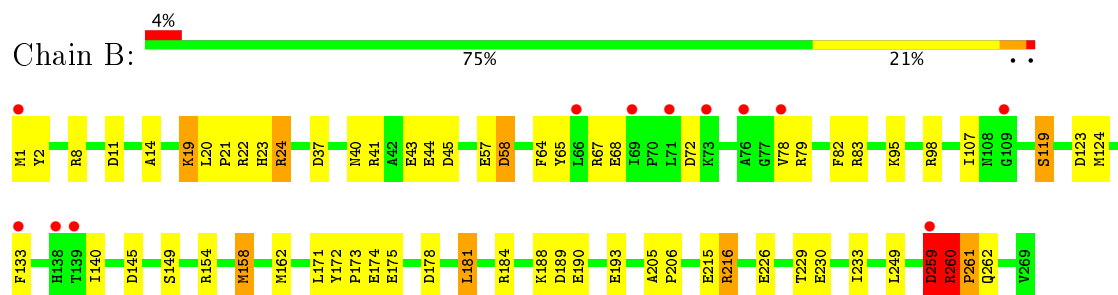
### 3 Residue-property plots

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.

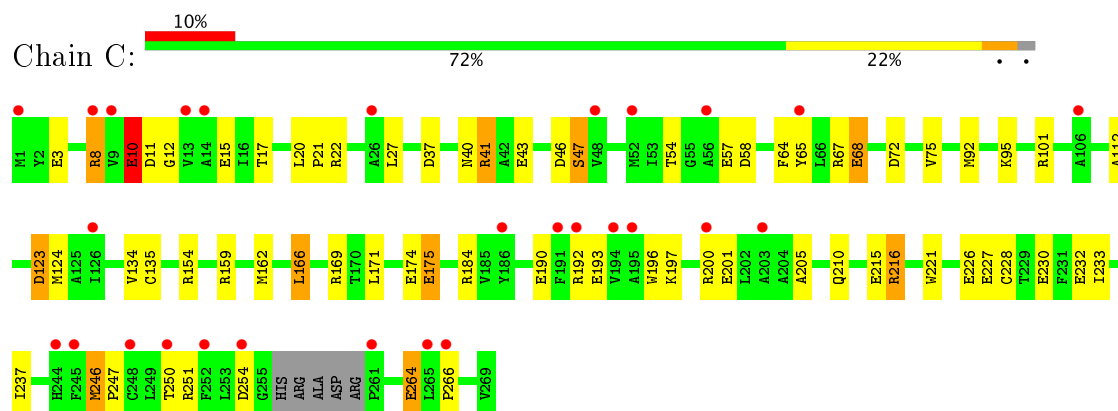
- Molecule 1: 4-chlorobenzoyl Coenzyme A dehalogenase



- Molecule 1: 4-chlorobenzoyl Coenzyme A dehalogenase



- Molecule 1: 4-chlorobenzoyl Coenzyme A dehalogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.10 Å   102.70 Å   90.70 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 1.90 46.38 – 1.68	Depositor EDS
% Data completeness (in resolution range)	88.0 (30.00-1.90) 79.9 (46.38-1.68)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 1.68 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.195 , (Not available) 0.298 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 90.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	7199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: PO4, CA, BCA

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	1.24	17/2139 (0.8%)	1.34	27/2898 (0.9%)
1	B	1.20	11/2153 (0.5%)	1.43	34/2916 (1.2%)
1	C	1.17	15/2100 (0.7%)	1.38	28/2843 (1.0%)
All	All	1.21	43/6392 (0.7%)	1.38	89/8657 (1.0%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	GLU	CD-OE2	11.35	1.38	1.25
1	A	68	GLU	CD-OE1	-10.57	1.14	1.25
1	A	57	GLU	CD-OE2	9.82	1.36	1.25
1	B	193	GLU	CD-OE2	9.35	1.35	1.25
1	A	190	GLU	CD-OE2	8.75	1.35	1.25
1	A	44	GLU	CD-OE2	8.22	1.34	1.25
1	A	175	GLU	CD-OE2	8.03	1.34	1.25
1	C	264	GLU	CD-OE2	7.83	1.34	1.25
1	A	43	GLU	CD-OE2	7.83	1.34	1.25
1	C	68	GLU	CD-OE2	7.80	1.34	1.25
1	B	175	GLU	CD-OE2	7.71	1.34	1.25
1	B	44	GLU	CD-OE2	7.61	1.34	1.25
1	A	226	GLU	CD-OE2	7.46	1.33	1.25
1	C	226	GLU	CD-OE2	7.20	1.33	1.25
1	C	3	GLU	CD-OE2	6.95	1.33	1.25
1	B	43	GLU	CD-OE1	-6.83	1.18	1.25
1	B	43	GLU	CD-OE2	6.79	1.33	1.25
1	B	230	GLU	CD-OE2	6.60	1.32	1.25
1	C	190	GLU	CD-OE2	6.57	1.32	1.25
1	A	232	GLU	CD-OE2	6.46	1.32	1.25
1	A	10	GLU	CD-OE2	6.39	1.32	1.25
1	B	215	GLU	CD-OE2	6.34	1.32	1.25
1	C	174	GLU	CD-OE2	6.30	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	CD-OE2	6.18	1.32	1.25
1	C	57	GLU	CD-OE2	6.12	1.32	1.25
1	B	174	GLU	CD-OE2	6.05	1.32	1.25
1	A	43	GLU	CD-OE1	-5.88	1.19	1.25
1	A	230	GLU	CD-OE2	5.82	1.32	1.25
1	C	230	GLU	CD-OE2	5.79	1.32	1.25
1	A	264	GLU	CD-OE2	5.71	1.31	1.25
1	A	68	GLU	CD-OE2	5.64	1.31	1.25
1	C	193	GLU	CD-OE2	5.64	1.31	1.25
1	C	10	GLU	CD-OE2	5.62	1.31	1.25
1	A	3	GLU	CD-OE2	5.58	1.31	1.25
1	C	227	GLU	CD-OE2	5.56	1.31	1.25
1	A	227	GLU	CD-OE2	5.55	1.31	1.25
1	B	190	GLU	CD-OE2	5.47	1.31	1.25
1	A	174	GLU	CD-OE2	5.40	1.31	1.25
1	C	43	GLU	CD-OE2	5.26	1.31	1.25
1	C	175	GLU	CD-OE1	-5.19	1.20	1.25
1	C	215	GLU	CD-OE2	5.18	1.31	1.25
1	A	193	GLU	CD-OE2	5.17	1.31	1.25
1	C	15	GLU	CD-OE2	5.17	1.31	1.25

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	B	216	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	A	72	ASP	CB-CG-OD1	8.97	126.37	118.30
1	B	145	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	C	169	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	189	ASP	CB-CG-OD2	-8.78	110.39	118.30
1	C	216	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	189	ASP	CB-CG-OD1	8.13	125.61	118.30
1	A	37	ASP	CB-CG-OD1	7.83	125.35	118.30
1	B	123	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	B	123	ASP	CB-CG-OD1	7.68	125.22	118.30
1	A	46	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	C	101	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	216	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	C	67	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	11	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	172	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	B	67	ARG	NE-CZ-NH1	7.43	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	C	123	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	B	154	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	C	123	ASP	CB-CG-OD1	7.26	124.83	118.30
1	C	200	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	259	ASP	CB-CG-OD1	7.17	124.75	118.30
1	C	46	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	A	11	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	46	ASP	CB-CG-OD1	6.86	124.47	118.30
1	C	251	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	72	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	B	41	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	257	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	C	159	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	C	251	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	58	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	184	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	259	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	41	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	C	184	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	154	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	200	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	192	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	216	ARG	CD-NE-CZ	6.12	132.16	123.60
1	C	184	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	259	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	B	11	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	37	ASP	CB-CG-OD2	-5.98	112.91	118.30
1	B	178	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	98	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	254	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	123	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	123	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	259	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	B	72	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	8	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	254	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	151	SER	N-CA-C	5.77	126.58	111.00
1	B	19	LYS	N-CA-CB	-5.77	100.22	110.60
1	C	37	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	22	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	58	ASP	CB-CG-OD2	-5.67	113.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	ASP	CB-CG-OD1	5.62	123.35	118.30
1	B	37	ASP	CB-CG-OD1	5.61	123.34	118.30
1	B	11	ASP	CB-CG-OD1	5.53	123.27	118.30
1	C	8	ARG	N-CA-CB	5.51	120.52	110.60
1	B	145	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	216	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	260	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	58	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	37	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	45	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	B	72	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	46	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	254	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	88	TRP	CA-CB-CG	-5.28	103.66	113.70
1	A	19	LYS	N-CA-CB	-5.26	101.13	110.60
1	B	98	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	184	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	159	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	72	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	260	ARG	CB-CA-C	-5.18	100.03	110.40
1	A	257	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	72	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	178	ASP	CB-CG-OD1	5.08	122.88	118.30
1	C	135	CYS	CA-CB-SG	-5.06	104.89	114.00
1	B	14	ALA	N-CA-CB	5.06	117.18	110.10
1	B	45	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	83	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	181	LEU	CA-CB-CG	-5.05	103.69	115.30
1	B	8	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	2088	0	2075	19	0
1	B	2097	0	2088	27	0
1	C	2051	0	2045	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	53	0	36	1	0
3	B	53	0	36	1	0
3	C	53	0	36	1	0
4	B	5	0	0	0	0
5	A	324	0	0	6	2
5	B	248	0	0	2	1
5	C	224	0	0	5	0
All	All	7199	0	6316	72	2

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 6.

All (72) 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:65:TYR:CD1	1:C:68:GLU:HG3	2.14	0.83
1:B:65:TYR:CD1	1:B:68:GLU:HG3	2.14	0.82
1:B:140:ILE:HG13	1:B:140:ILE:O	1.94	0.68
1:C:41:ARG:NH1	5:C:457:HOH:O	2.25	0.68
1:A:21:PRO:HD2	5:A:591:HOH:O	1.97	0.64
1:A:75:VAL:HG22	5:B:423:HOH:O	1.98	0.64
1:C:171:LEU:HD11	1:C:175:GLU:HG2	1.80	0.63
1:A:140:ILE:O	1:A:140:ILE:HG13	2.01	0.61
1:B:1:MET:HG2	1:B:2:TYR:N	2.17	0.59
5:A:533:HOH:O	1:C:75:VAL:HG22	2.01	0.59
1:C:10:GLU:HG2	1:C:196:TRP:CZ3	2.37	0.59
1:C:264:GLU:O	1:C:266:PRO:HD3	2.03	0.59
1:B:229:THR:O	1:B:233:ILE:HG13	2.03	0.58
1:C:162:MET:HG3	1:C:166:LEU:HD22	1.85	0.57
1:C:10:GLU:HG2	1:C:196:TRP:CH2	2.38	0.57
1:C:197:LYS:HB3	5:C:331:HOH:O	2.04	0.56
1:B:260:ARG:HB3	1:B:261:PRO:HD2	1.89	0.54
1:B:40:ASN:OD1	1:B:95:LYS:HE3	2.07	0.54
1:B:259:ASP:OD2	1:B:260:ARG:HG3	2.08	0.54
1:C:20:LEU:N	1:C:21:PRO:HD3	2.24	0.53
1:B:259:ASP:C	1:B:260:ARG:HG3	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PHE:HB2	3:B:272:BCA:C2B	2.40	0.52
1:A:9:VAL:HG22	1:A:14:ALA:HA	1.91	0.52
1:A:246:MET:HG2	5:A:533:HOH:O	2.10	0.52
1:A:8:ARG:NH2	1:A:196:TRP:CE2	2.79	0.51
1:C:228:CYS:O	1:C:232:GLU:HG3	2.11	0.50
1:B:58:ASP:HB2	5:B:488:HOH:O	2.11	0.50
1:B:107:ILE:HD11	1:B:119[A]:SER:HB3	1.94	0.49
1:B:23:HIS:O	1:B:24:ARG:HB2	2.13	0.49
1:C:196:TRP:HB3	5:C:353:HOH:O	2.12	0.49
1:A:139:THR:HG21	5:A:420:HOH:O	2.11	0.49
1:A:20:LEU:N	1:A:21:PRO:HD3	2.28	0.48
1:C:64:PHE:HB2	3:C:271:BCA:C2B	2.43	0.48
1:B:133:PHE:HB2	1:B:171:LEU:HB3	1.95	0.48
1:A:90:GLN:HG2	1:A:94:HIS:CE1	2.49	0.47
1:C:22:ARG:HG2	5:C:334:HOH:O	2.14	0.47
1:A:137:TRP:CD1	1:A:144:ASN:HA	2.48	0.47
1:C:197:LYS:O	1:C:201:GLU:HG3	2.14	0.47
1:C:246:MET:O	1:C:250:THR:HG23	2.14	0.47
1:B:172:TYR:HB3	1:B:173:PRO:HD2	1.96	0.47
1:A:163:GLU:OE2	5:A:553:HOH:O	2.20	0.47
1:B:20:LEU:N	1:B:21:PRO:HD3	2.29	0.47
1:C:27:LEU:HD13	1:C:92:MET:HE1	1.97	0.47
1:B:162:MET:HG2	1:C:123:ASP:O	2.16	0.46
1:C:12:GLY:HA2	1:C:47:SER:O	2.15	0.45
1:B:205:ALA:HB1	1:B:206:PRO:HD2	1.98	0.45
1:C:40:ASN:OD1	1:C:95:LYS:HE3	2.16	0.45
1:A:64:PHE:HB2	3:A:271:BCA:C2B	2.47	0.44
1:C:205:ALA:HB3	1:C:210:GLN:NE2	2.32	0.44
1:B:58:ASP:CG	1:B:188:LYS:HZ1	2.20	0.44
1:C:17:THR:HA	1:C:54:THR:O	2.17	0.44
1:C:233:ILE:O	1:C:237:ILE:HG12	2.18	0.43
1:A:8:ARG:HE	1:A:196:TRP:HZ2	1.65	0.43
1:B:20:LEU:N	1:B:21:PRO:CD	2.81	0.43
1:B:260:ARG:HB3	1:B:261:PRO:CD	2.48	0.43
1:A:31:ALA:O	1:A:35:VAL:HG23	2.19	0.43
5:A:520:HOH:O	1:B:262:GLN:HG2	2.18	0.43
1:B:95:LYS:HA	1:B:95:LYS:HD3	1.79	0.43
1:C:20:LEU:N	1:C:21:PRO:CD	2.78	0.42
1:B:158:MET:O	1:B:158:MET:HG3	2.18	0.42
1:A:140:ILE:HD11	1:B:249:LEU:HA	2.02	0.42
1:B:78:VAL:O	1:B:82:PHE:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ARG:HG2	1:C:221:TRP:CE2	2.55	0.41
1:A:149:SER:CB	1:B:216:ARG:HB3	2.50	0.41
1:C:124:MET:HE3	1:C:124:MET:HB3	1.69	0.41
1:B:149:SER:CB	1:C:216:ARG:HB3	2.50	0.41
1:C:112:ALA:HA	1:C:134:VAL:O	2.20	0.41
1:A:20:LEU:N	1:A:21:PRO:CD	2.82	0.41
1:A:8:ARG:NH2	1:A:196:TRP:CZ2	2.89	0.41
1:C:246:MET:CB	1:C:247:PRO:HD3	2.51	0.41
1:A:89:TRP:CH2	1:A:114:GLY:HA3	2.55	0.41
1:C:41:ARG:NH2	5:C:439:HOH:O	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:438:HOH:O	5:B:403:HOH:O[2_575]	2.11	0.09
5:A:356:HOH:O	5:A:423:HOH:O[3_546]	2.14	0.06

## 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	267/269 (99%)	258 (97%)	9 (3%)	0	100	100
1	B	269/269 (100%)	257 (96%)	12 (4%)	0	100	100
1	C	261/269 (97%)	250 (96%)	11 (4%)	0	100	100
All	All	797/807 (99%)	765 (96%)	32 (4%)	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	214/214 (100%)	213 (100%)	1 (0%)	91	91
1	B	216/214 (101%)	204 (94%)	12 (6%)	25	13
1	C	211/214 (99%)	205 (97%)	6 (3%)	49	40
All	All	641/642 (100%)	622 (97%)	19 (3%)	49	37

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	B	19	LYS
1	B	24	ARG
1	B	79	ARG
1	B	83	ARG
1	B	119[A]	SER
1	B	119[B]	SER
1	B	124	MET
1	B	158	MET
1	B	181	LEU
1	B	259	ASP
1	B	260	ARG
1	B	261	PRO
1	C	8	ARG
1	C	10	GLU
1	C	41	ARG
1	C	47	SER
1	C	166	LEU
1	C	246	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	210	GLN
1	B	33	GLN
1	B	235	ASN
1	C	33	GLN
1	C	90	GLN
1	C	235	ASN

### 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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	BCA	A	271	-	49,56,60	1.77	5 (10%)	56,82,89	1.53	8 (14%)
4	PO4	B	271	-	4,4,4	1.72	2 (50%)	6,6,6	0.56	0
3	BCA	B	272	-	49,56,60	2.04	6 (12%)	56,82,89	2.42	12 (21%)
3	BCA	C	271	-	49,56,60	1.71	8 (16%)	56,82,89	1.74	11 (19%)

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
3	BCA	A	271	-	-	0/46/66/71	0/4/4/4
4	PO4	B	271	-	-	0/0/0/0	0/0/0/0
3	BCA	B	272	-	-	0/46/66/71	0/4/4/4
3	BCA	C	271	-	-	0/46/66/71	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	272	BCA	C2B-C1B	-6.01	1.37	1.49
3	C	271	BCA	O4D-C1D	-3.30	1.36	1.41
4	B	271	PO4	P-O2	-2.24	1.46	1.54
4	B	271	PO4	P-O3	-2.21	1.46	1.54
3	C	271	BCA	C6B-C5B	2.09	1.43	1.38
3	A	271	BCA	OAP-CAP	2.16	1.46	1.42
3	B	272	BCA	C1B-S1P	2.23	1.81	1.76
3	C	271	BCA	O2B-C5B	2.23	1.42	1.37
3	C	271	BCA	C4B-C5B	2.43	1.43	1.38
3	C	271	BCA	C2A-N1A	2.47	1.38	1.33
3	A	271	BCA	C6P-C5P	2.49	1.56	1.51
3	B	272	BCA	C6B-C5B	2.62	1.44	1.38
3	A	271	BCA	C7B-C6B	2.67	1.43	1.38
3	C	271	BCA	C7B-C2B	2.72	1.43	1.39
3	B	272	BCA	C4B-C5B	3.11	1.45	1.38
3	C	271	BCA	C5P-N4P	5.87	1.47	1.33
3	B	272	BCA	C5P-N4P	5.91	1.47	1.33
3	C	271	BCA	C9P-N8P	6.12	1.46	1.33
3	A	271	BCA	C5P-N4P	6.37	1.48	1.33
3	A	271	BCA	C9P-N8P	7.34	1.48	1.33
3	B	272	BCA	C9P-N8P	8.51	1.51	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	272	BCA	CEP-CBP-CAP	-7.54	95.74	108.82
3	B	272	BCA	C3P-N4P-C5P	-6.26	110.82	122.84
3	A	271	BCA	C7P-N8P-C9P	-6.02	111.36	122.59
3	A	271	BCA	C3P-N4P-C5P	-5.29	112.69	122.84
3	C	271	BCA	C7P-N8P-C9P	-5.23	112.83	122.59
3	C	271	BCA	C3P-N4P-C5P	-4.94	113.35	122.84
3	B	272	BCA	C7P-N8P-C9P	-4.80	113.64	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	271	BCA	CEP-CBP-CAP	-3.65	102.49	108.82
3	C	271	BCA	CAP-C9P-N8P	-3.51	109.27	116.58
3	B	272	BCA	O5P-C5P-N4P	-2.86	117.52	122.97
3	C	271	BCA	O6A-CCP-CBP	-2.73	106.16	110.55
3	A	271	BCA	C6P-C5P-N4P	-2.57	112.06	116.49
3	C	271	BCA	C6P-C5P-N4P	-2.55	112.10	116.49
3	B	272	BCA	CAP-C9P-N8P	-2.48	111.43	116.58
3	B	272	BCA	C6P-C5P-N4P	-2.26	112.59	116.49
3	C	271	BCA	C4B-C3B-C2B	-2.26	118.26	120.79
3	A	271	BCA	P2A-O6A-CCP	-2.19	107.73	121.57
3	A	271	BCA	C2P-C3P-N4P	-2.18	107.69	112.49
3	B	272	BCA	C4B-C3B-C2B	-2.13	118.41	120.79
3	A	271	BCA	CDP-CBP-CAP	2.07	112.41	108.82
3	A	271	BCA	C5A-C6A-N6A	2.11	124.76	120.47
3	C	271	BCA	O5A-P2A-O6A	2.11	118.12	108.14
3	B	272	BCA	CEP-CBP-CCP	2.42	111.92	108.37
3	C	271	BCA	C2P-S1P-C1B	2.55	102.81	99.68
3	B	272	BCA	C7B-C2B-C3B	2.55	122.11	118.58
3	C	271	BCA	C5A-C6A-N6A	3.02	126.62	120.47
3	A	271	BCA	C2P-S1P-C1B	3.35	103.79	99.68
3	C	271	BCA	CDP-CBP-CAP	4.67	116.92	108.82
3	B	272	BCA	O5A-P2A-O6A	5.13	132.35	108.14
3	B	272	BCA	C2P-S1P-C1B	7.10	108.40	99.68
3	B	272	BCA	CDP-CBP-CAP	7.65	122.08	108.82

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	A	271	BCA	1	0
3	B	272	BCA	1	0
3	C	271	BCA	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	268/269 (99%)	0.09	1 (0%) 92 93	6, 13, 35, 60	0
1	B	269/269 (100%)	0.61	12 (4%) 34 37	5, 16, 46, 92	0
1	C	264/269 (98%)	1.02	28 (10%) 7 8	7, 18, 52, 78	0
All	All	801/807 (99%)	0.57	41 (5%) 29 32	5, 15, 46, 92	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.6
1	C	1	MET	3.6
1	C	266	PRO	3.0
1	C	194	VAL	3.0
1	C	261	PRO	2.9
1	B	66	LEU	2.8
1	C	200	ARG	2.8
1	C	56	ALA	2.7
1	C	192	ARG	2.7
1	B	259	ASP	2.6
1	B	78	VAL	2.6
1	C	191	PHE	2.6
1	C	265	LEU	2.6
1	A	258	ALA	2.6
1	C	244	HIS	2.5
1	C	9	VAL	2.5
1	C	106	ALA	2.5
1	C	252	PHE	2.4
1	B	69	ILE	2.4
1	C	14	ALA	2.4
1	B	71	LEU	2.3
1	C	245	PHE	2.3
1	C	126	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	109	GLY	2.3
1	C	195	ALA	2.3
1	B	73	LYS	2.3
1	C	254	ASP	2.2
1	C	65	TYR	2.2
1	C	26	ALA	2.2
1	B	133	PHE	2.2
1	C	13	VAL	2.2
1	B	139	THR	2.1
1	C	250	THR	2.1
1	C	52	MET	2.1
1	B	76	ALA	2.1
1	C	48	VAL	2.1
1	C	8	ARG	2.0
1	C	186	TYR	2.0
1	B	138	HIS	2.0
1	C	203	ALA	2.0
1	C	248	CYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	B	271	5/5	0.81	0.33	4.25	47,53,80,100	0
3	BCA	C	271	53/57	0.85	0.16	0.24	8,16,28,39	0
3	BCA	B	272	53/57	0.82	0.17	0.02	10,25,51,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BCA	A	271	53/57	0.94	0.11	-0.17	6,14,23,31	0
2	CA	B	270	1/1	0.90	0.11	-0.50	13,13,13,13	0
2	CA	C	270	1/1	0.86	0.14	-1.12	23,23,23,23	0
2	CA	A	270	1/1	0.93	0.09	-1.95	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.