



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:24 PM GMT

PDB ID : 3R75
Title : Crystal structure of 2-amino-2-desoxyisochorismate synthase (ADIC) synthase PhzE from Burkholderia lata 383 in complex with benzoate, pyruvate, glutamine and contaminating Zn²⁺
Authors : Li, Q.A.; Mavrodi, D.V.; Thomashow, L.S.; Roessle, M.; Blankenfeldt, W.
Deposited on : 2011-03-22
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

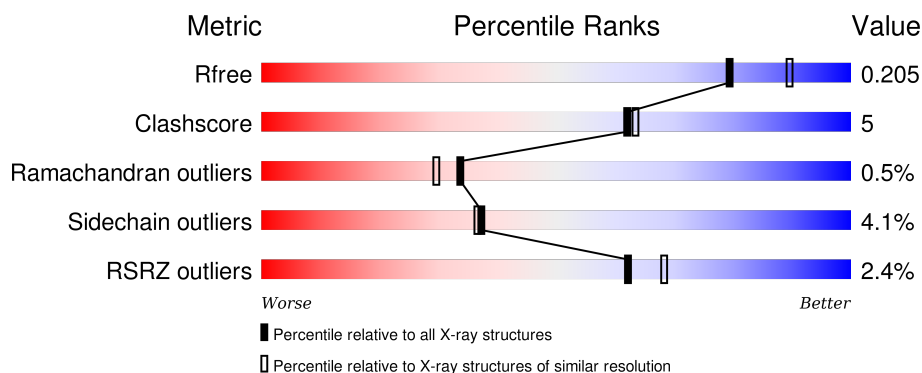
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

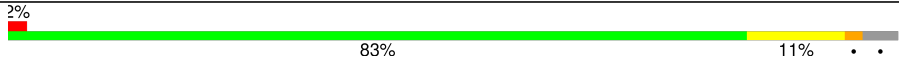
The reported resolution of this entry is 2.10 Å.

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	645	 3% 83% 11% • •
1	B	645	 2% 83% 11% • •

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
5	PO4	A	900	-	-	-	X
5	PO4	B	900	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10496 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 Anthranilate/para-aminobenzoate synthases component I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	21	0
			4822	3028	870	897	27			
1	B	622	Total	C	N	O	S	0	20	0
			4841	3035	866	913	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q396C7
A	0	HIS	-	EXPRESSION TAG	UNP Q396C7
B	-1	GLY	-	EXPRESSION TAG	UNP Q396C7
B	0	HIS	-	EXPRESSION TAG	UNP Q396C7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

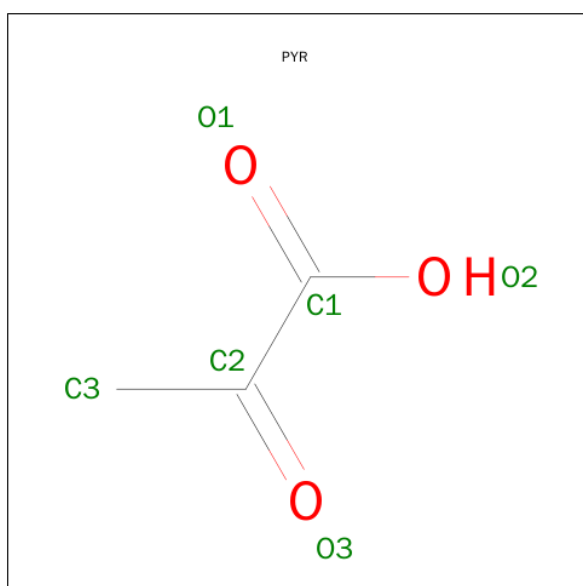
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



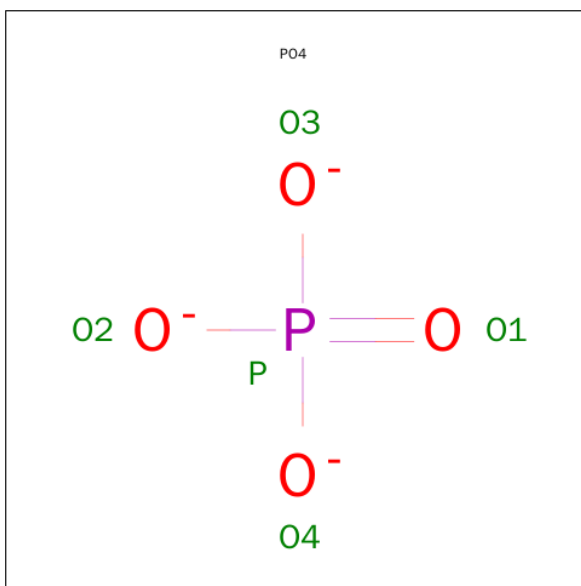
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		
3	B	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	1		

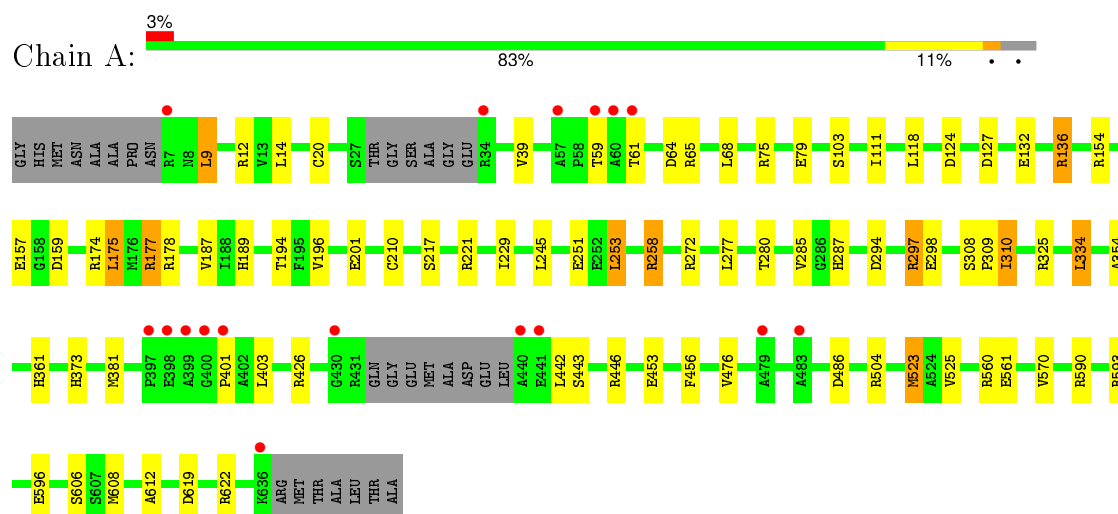
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	396	Total	O	0	0
			396	396		
7	B	392	Total	O	0	0
			392	392		

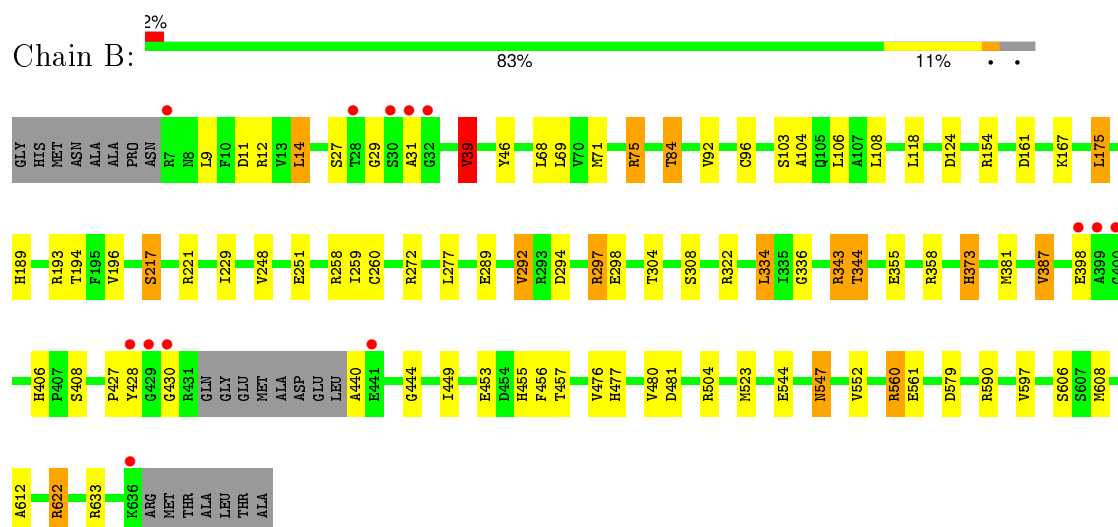
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Anthranilate/para-aminobenzoate synthases component I



- Molecule 1: Anthranilate/para-aminobenzoate synthases component I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	259.71 Å 94.51 Å 53.55 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.10 19.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.62-2.10) 99.5 (19.86-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 2.09 Å)	Xtriage
Refinement program	REFMAC 5.6.0077	Depositor
R, R_{free}	0.147 , 0.200 0.155 , 0.205	Depositor DCC
R_{free} test set	3934 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 77637 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10496	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, PO4, ZN, BEZ, CYG, PYR

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	1.01	2/4966 (0.0%)	1.06	31/6736 (0.5%)
1	B	1.00	6/4978 (0.1%)	1.07	28/6756 (0.4%)
All	All	1.00	8/9944 (0.1%)	1.07	59/13492 (0.4%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	504	ARG	CD-NE	-7.08	1.34	1.46
1	A	20	CYS	CB-SG	-6.88	1.70	1.82
1	B	504	ARG	CD-NE	-6.51	1.35	1.46
1	B	633	ARG	CD-NE	-6.01	1.36	1.46
1	B	597	VAL	CB-CG2	6.00	1.65	1.52
1	B	96	CYS	CB-SG	5.89	1.92	1.82
1	B	196	VAL	CB-CG2	-5.25	1.41	1.52
1	B	552	VAL	CB-CG2	5.04	1.63	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	ARG	NE-CZ-NH2	-15.48	112.56	120.30
1	B	633	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	A	504	ARG	NE-CZ-NH2	-14.45	113.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-13.01	113.79	120.30
1	A	297	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	B	297	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	B	622	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	A	177	ARG	NE-CZ-NH1	11.25	125.93	120.30
1	B	504	ARG	NE-CZ-NH1	10.91	125.75	120.30
1	B	154	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	297	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	A	504	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	B	297	ARG	NE-CZ-NH1	10.11	125.35	120.30
1	B	633	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	B	622	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	154	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	154	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	154	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	12	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	272	ARG	NE-CZ-NH1	-7.31	116.65	120.30
1	B	633	ARG	CG-CD-NE	-6.95	97.20	111.80
1	B	590	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	253[A]	LEU	CB-CG-CD1	6.65	122.31	111.00
1	A	253[B]	LEU	CB-CG-CD1	6.65	122.31	111.00
1	B	387	VAL	CG1-CB-CG2	6.59	121.44	110.90
1	B	504	ARG	CG-CD-NE	-6.37	98.43	111.80
1	B	175	LEU	CB-CG-CD1	6.13	121.42	111.00
1	A	258	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	B	124	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	177	ARG	CD-NE-CZ	5.98	131.97	123.60
1	A	504	ARG	CG-CD-NE	-5.95	99.31	111.80
1	A	12	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	426	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	68	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	B	39	VAL	CG1-CB-CG2	5.79	120.16	110.90
1	B	343	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	334	LEU	CB-CG-CD1	5.71	120.72	111.00
1	A	68	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	258	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	127	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	622	ARG	CG-CD-NE	-5.43	100.40	111.80
1	A	64	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	590	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	12	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	221	ARG	NE-CZ-NH2	-5.32	117.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	124	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	68	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	253[A]	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	253[B]	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	590	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	221	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	560	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	177	ARG	CG-CD-NE	-5.10	101.09	111.80
1	B	343	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	325	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	124	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	136[A]	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	A	136[B]	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	444	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4822	0	4783	49	0
1	B	4841	0	4797	59	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
4	A	6	0	3	0	0
4	B	6	0	3	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	396	0	0	7	0
7	B	392	0	0	10	0
All	All	10496	0	9596	105	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.

All (105) 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:248[B]:VAL:HG21	1:B:304:THR:HG22	1.24	1.18
1:B:440:ALA:HB2	7:B:656:HOH:O	1.55	1.03
1:B:248[B]:VAL:HG21	1:B:304:THR:CG2	1.88	1.01
1:B:344:THR:HG21	7:B:694:HOH:O	1.61	1.00
1:B:71:MET:HB2	1:B:92[B]:VAL:HG23	1.49	0.92
1:B:75:ARG:HA	1:B:84:THR:HG21	1.53	0.88
1:B:477:HIS:ND1	7:B:778:HOH:O	2.10	0.85
1:A:59:THR:OG1	1:A:65:ARG:NH2	2.14	0.80
1:B:344:THR:HG23	7:B:670:HOH:O	1.81	0.79
1:A:258:ARG:NH2	1:A:298:GLU:OE1	2.16	0.79
1:B:608[B]:MET:HE3	1:B:612:ALA:H	1.50	0.76
1:B:258:ARG:NH2	1:B:298:GLU:OE1	2.18	0.75
1:B:71:MET:HB2	1:B:92[B]:VAL:CG2	2.16	0.74
1:A:210[A]:CYS:SG	1:A:287[A]:HIS:HE1	2.12	0.73
1:A:523[A]:MET:HE1	1:A:525:VAL:HG22	1.72	0.71
1:A:9:LEU:HD13	1:A:39[B]:VAL:HG22	1.72	0.70
1:A:608[B]:MET:HE3	1:A:612:ALA:H	1.56	0.69
1:B:248[B]:VAL:CG2	1:B:304:THR:CG2	2.69	0.68
1:A:210[A]:CYS:SG	1:A:287[A]:HIS:CE1	2.87	0.67
1:A:608[B]:MET:CE	1:A:612:ALA:H	2.08	0.67
1:B:9:LEU:HD23	1:B:39:VAL:HG22	1.79	0.65
1:B:27:SER:HA	7:B:943:HOH:O	1.95	0.65
1:A:277:LEU:C	1:A:277:LEU:HD12	2.18	0.64
1:B:161:ASP:O	1:B:167:LYS:NZ	2.28	0.64
7:A:991:HOH:O	1:B:106:LEU:HD22	1.98	0.64
1:B:336:GLY:C	1:B:344:THR:HG22	2.18	0.63
1:B:381[B]:MET:HE3	7:B:855:HOH:O	2.00	0.60
1:B:608[B]:MET:CE	1:B:612:ALA:H	2.14	0.60
1:A:523[A]:MET:CE	1:A:525:VAL:HG22	2.31	0.60
1:B:27:SER:HB2	7:B:772:HOH:O	2.03	0.58
7:A:991:HOH:O	1:B:106:LEU:CD2	2.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:HIS:HD2	1:B:408[B]:SER:H	1.49	0.58
1:A:523[A]:MET:HE3	1:A:525:VAL:CG2	2.33	0.58
1:B:406:HIS:HD2	1:B:408[A]:SER:H	1.49	0.58
1:B:427:PRO:O	1:B:430:GLY:HA3	2.04	0.57
1:A:381[A]:MET:HE1	7:A:959:HOH:O	2.05	0.57
1:A:523[A]:MET:CE	1:A:525:VAL:CG2	2.83	0.56
1:A:174:ARG:O	1:A:178[B]:ARG:HG2	2.05	0.56
1:A:570:VAL:HG21	1:A:596:GLU:CG	2.35	0.56
1:A:132:GLU:OE1	1:A:136[B]:ARG:HD3	2.07	0.54
1:B:248[B]:VAL:CG2	1:B:304:THR:HG23	2.36	0.54
1:B:579:ASP:HB2	7:B:986:HOH:O	2.06	0.54
1:A:403:LEU:HD22	1:B:229:ILE:HD13	1.91	0.53
1:A:9:LEU:HD13	1:A:39[B]:VAL:CG2	2.39	0.53
1:B:277:LEU:HD12	1:B:277:LEU:C	2.29	0.52
1:A:310:ILE:HD12	1:A:310:ILE:O	2.10	0.52
1:A:210[B]:CYS:SG	1:A:285[B]:VAL:CG1	2.99	0.52
1:B:449:ILE:HG21	1:B:457[A]:THR:HG23	1.92	0.51
1:A:159:ASP:OD1	1:A:361[A]:HIS:HD2	1.94	0.51
1:A:523[B]:MET:HA	1:A:606:SER:O	2.12	0.50
1:B:336:GLY:CA	1:B:344:THR:HG22	2.42	0.50
1:B:480:VAL:HG12	1:B:481:ASP:H	1.77	0.49
1:A:561:GLU:OE2	1:A:622[A]:ARG:NH2	2.46	0.49
1:B:71:MET:CB	1:B:92[B]:VAL:HG23	2.34	0.49
1:A:210[B]:CYS:SG	1:A:285[B]:VAL:HG13	2.52	0.48
1:B:480:VAL:HG12	1:B:481:ASP:N	2.29	0.48
1:A:196[B]:VAL:HG23	1:A:354:ALA:HB3	1.96	0.48
1:B:561:GLU:OE2	1:B:622:ARG:NH2	2.38	0.48
1:A:187:VAL:HB	1:A:196[B]:VAL:HG12	1.96	0.48
1:B:193:ARG:NH1	1:B:355:GLU:OE2	2.40	0.47
1:B:523[A]:MET:HA	1:B:606:SER:O	2.14	0.47
1:A:277:LEU:O	1:A:277:LEU:HD12	2.15	0.47
1:A:523[A]:MET:HA	1:A:606:SER:O	2.14	0.47
1:B:406:HIS:CD2	1:B:408[A]:SER:H	2.30	0.47
1:B:406:HIS:CD2	1:B:408[B]:SER:H	2.29	0.47
1:B:217:SER:HB2	1:B:248[A]:VAL:HG21	1.98	0.46
1:B:27:SER:CA	7:B:943:HOH:O	2.58	0.46
1:A:403:LEU:CD2	1:B:229:ILE:HD13	2.45	0.46
1:B:46:TYR:CE1	1:B:92[B]:VAL:HG12	2.50	0.46
1:B:46:TYR:CE1	1:B:92[B]:VAL:CG1	2.99	0.46
1:A:189:HIS:HD2	1:A:194:THR:OG1	1.99	0.46
1:B:9:LEU:CD2	1:B:39:VAL:HG22	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:HD13	1:B:334:LEU:HD13	1.98	0.46
1:B:272:ARG:HH22	5:B:900:PO4:P	2.39	0.45
1:B:294:ASP:OD1	1:B:297:ARG:NH2	2.49	0.45
1:A:251:GLU:CD	1:A:308:SER:CB	2.85	0.45
1:B:292[A]:VAL:HG13	1:B:343:ARG:HG2	1.98	0.45
1:A:9:LEU:HD13	1:A:39[A]:VAL:HG12	1.97	0.45
1:A:157:GLU:OE2	1:A:361[A]:HIS:HE1	2.00	0.45
1:A:61:THR:HG23	1:A:65:ARG:NH1	2.32	0.45
1:A:294:ASP:OD1	1:A:297:ARG:NH2	2.50	0.44
1:A:308:SER:HA	1:A:309:PRO:C	2.37	0.44
1:A:258:ARG:HD2	1:B:455:HIS:CG	2.52	0.44
1:A:285[B]:VAL:HG23	7:A:835:HOH:O	2.18	0.44
1:A:619:ASP:OD2	1:A:622[A]:ARG:NH1	2.51	0.44
1:A:245:LEU:HD22	1:A:280:THR:HB	2.01	0.43
1:B:259[A]:ILE:HG22	1:B:260:CYS:SG	2.59	0.43
1:A:136[A]:ARG:HD3	7:A:693:HOH:O	2.19	0.43
1:B:547:ASN:HD22	1:B:547:ASN:HA	1.66	0.43
1:A:132:GLU:O	1:A:136[B]:ARG:HG2	2.19	0.42
1:A:229:ILE:HG22	7:A:822:HOH:O	2.18	0.42
1:B:14:LEU:HA	1:B:14:LEU:HD12	1.82	0.42
1:B:189:HIS:HD2	1:B:194:THR:OG1	2.03	0.41
1:A:446:ARG:HD3	1:A:486:ASP:OD1	2.19	0.41
1:B:373:HIS:N	1:B:373:HIS:ND1	2.67	0.41
1:B:248[B]:VAL:CG2	1:B:304:THR:HG22	2.18	0.41
1:A:14:LEU:HD11	1:A:111:ILE:HG12	2.02	0.41
1:A:201:GLU:OE1	7:A:660:HOH:O	2.22	0.41
1:A:132:GLU:OE1	1:A:136[B]:ARG:CD	2.69	0.41
1:B:322:ARG:HD3	7:B:649:HOH:O	2.20	0.41
1:A:79:GLU:OE1	1:A:297:ARG:HD3	2.21	0.41
1:B:217:SER:HB2	1:B:248[B]:VAL:HG11	2.03	0.41
1:A:277:LEU:C	1:A:277:LEU:CD1	2.88	0.41
1:B:251:GLU:CD	1:B:308:SER:CB	2.89	0.40
1:B:104:ALA:O	1:B:108:LEU:HG	2.21	0.40

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	630/645 (98%)	610 (97%)	18 (3%)	2 (0%)	46	45
1	B	637/645 (99%)	617 (97%)	16 (2%)	4 (1%)	30	24
All	All	1267/1290 (98%)	1227 (97%)	34 (3%)	6 (0%)	34	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	PRO
1	B	31	ALA
1	B	453	GLU
1	A	453	GLU
1	B	428	TYR
1	B	29	GLY

5.3.2 Protein sidechains [i](#)

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	503/506 (99%)	483 (96%)	20 (4%)	38	38
1	B	507/506 (100%)	484 (96%)	23 (4%)	34	32
All	All	1010/1012 (100%)	967 (96%)	43 (4%)	37	34

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	75	ARG
1	A	103	SER
1	A	118	LEU
1	A	175	LEU
1	A	177	ARG
1	A	217	SER
1	A	253[A]	LEU
1	A	253[B]	LEU
1	A	310	ILE
1	A	334	LEU
1	A	373	HIS
1	A	442	LEU
1	A	443	SER
1	A	456	PHE
1	A	476	VAL
1	A	523[A]	MET
1	A	523[B]	MET
1	A	560	ARG
1	A	593	ARG
1	B	11	ASP
1	B	14	LEU
1	B	39	VAL
1	B	75	ARG
1	B	84	THR
1	B	103	SER
1	B	118	LEU
1	B	175	LEU
1	B	217	SER
1	B	289	GLU
1	B	292[A]	VAL
1	B	292[B]	VAL
1	B	334	LEU
1	B	344	THR
1	B	358	ARG
1	B	373	HIS
1	B	387	VAL
1	B	398	GLU
1	B	456	PHE
1	B	476	VAL
1	B	544	GLU
1	B	547	ASN
1	B	560	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	189	HIS
1	A	392	ASN
1	A	547	ASN
1	B	66	GLN
1	B	189	HIS
1	B	406	HIS
1	B	462	GLN
1	B	547	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CYG	A	526	1,6	10,14,15	3.63	2 (20%)	6,17,19	6.39	5 (83%)
1	CYG	B	526	1,6	10,14,15	3.80	2 (20%)	6,17,19	6.81	5 (83%)

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
1	CYG	A	526	1,6	-	0/10/16/18	0/0/0/0
1	CYG	B	526	1,6	-	0/10/16/18	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	CYG	OE2-CD1	2.55	1.25	1.21
1	A	526	CYG	OE2-CD1	3.17	1.26	1.21
1	A	526	CYG	CD1-SG	10.63	1.98	1.76
1	B	526	CYG	CD1-SG	11.52	2.00	1.76

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	CYG	OE2-CD1-CG1	-13.03	114.97	123.94
1	A	526	CYG	OE2-CD1-CG1	-12.10	115.61	123.94
1	A	526	CYG	CB1-CG1-CD1	-6.62	103.34	113.12
1	B	526	CYG	CB1-CG1-CD1	-6.33	103.77	113.12
1	A	526	CYG	O-C-CA	-2.82	118.16	125.49
1	B	526	CYG	O-C-CA	-2.75	118.33	125.49
1	B	526	CYG	OE2-CD1-SG	2.92	125.15	122.83
1	A	526	CYG	OE2-CD1-SG	4.08	126.07	122.83
1	A	526	CYG	CG1-CD1-SG	5.50	118.30	113.36
1	B	526	CYG	CG1-CD1-SG	7.22	119.85	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	BEZ	A	701	2	6,9,9	0.71	0	8,11,11	0.75	0
4	PYR	A	702	-	2,5,5	0.29	0	2,6,6	1.06	0
5	PO4	A	900	-	4,4,4	1.89	1 (25%)	6,6,6	0.41	0
3	BEZ	B	701	2	6,9,9	0.59	0	8,11,11	1.24	0
4	PYR	B	702	-	2,5,5	0.54	0	2,6,6	1.61	0
5	PO4	B	900	-	4,4,4	0.25	0	6,6,6	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEZ	A	701	2	-	0/0/4/4	0/1/1/1
4	PYR	A	702	-	-	0/0/4/4	0/0/0/0
5	PO4	A	900	-	-	0/0/0/0	0/0/0/0
3	BEZ	B	701	2	-	0/0/4/4	0/1/1/1
4	PYR	B	702	-	-	0/0/4/4	0/0/0/0
5	PO4	B	900	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	PO4	P-O3	-3.57	1.40	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	900	PO4	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, 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	615/645 (95%)	-0.26	17 (2%) 56 64	22, 36, 62, 117	0
1	B	621/645 (96%)	-0.29	13 (2%) 67 72	24, 36, 61, 89	0
All	All	1236/1290 (95%)	-0.28	30 (2%) 62 68	22, 36, 62, 117	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	GLY	11.5
1	A	399	ALA	7.7
1	A	440	ALA	5.7
1	B	32	GLY	5.5
1	B	31	ALA	4.6
1	A	398	GLU	4.3
1	B	428	TYR	4.2
1	B	430	GLY	4.0
1	B	7	ARG	4.0
1	A	60	ALA	3.7
1	B	636	LYS	3.6
1	A	34	ARG	3.5
1	B	28	THR	3.5
1	B	429	GLY	3.4
1	A	59	THR	3.1
1	A	430	GLY	3.0
1	B	399	ALA	3.0
1	A	397	PRO	2.9
1	A	441	GLU	2.9
1	A	636	LYS	2.8
1	A	401	PRO	2.8
1	B	30	SER	2.8
1	B	441	GLU	2.7
1	A	61	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	57	ALA	2.4
1	B	400	GLY	2.4
1	B	398	GLU	2.3
1	A	7	ARG	2.2
1	A	483	ALA	2.1
1	A	479	ALA	2.1

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

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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CYG	B	526	15/16	0.97	0.10	-	25,29,32,36	0
1	CYG	A	526	15/16	0.95	0.10	-	29,34,39,48	0

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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	PO4	B	900	5/5	0.94	0.33	5.51	60,75,94,103	0
5	PO4	A	900	5/5	0.93	0.34	4.82	13,15,18,25	5
2	MG	A	700	1/1	0.99	0.10	-0.07	26,26,26,26	0
3	BEZ	A	701	9/9	0.98	0.09	-0.11	23,27,30,31	0
4	PYR	A	702	6/6	0.97	0.08	-0.30	30,33,38,45	0
3	BEZ	B	701	9/9	0.96	0.08	-0.31	28,30,33,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PYR	B	702	6/6	0.99	0.06	-1.20	30,32,38,40	0
2	MG	B	700	1/1	0.96	0.06	-1.26	28,28,28,28	0
6	ZN	B	950	1/1	1.00	0.05	-	47,47,47,47	1
6	ZN	A	950	1/1	0.99	0.03	-	51,51,51,51	1
2	MG	B	644	1/1	0.87	0.10	-	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.