Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:23 PM GMT

PDB ID	:	3R76
Title	:	Crystal structure of 2-amino-2-desoxyisochorismate synthase (ADIC) synthase PhzE from Burkholderia lata 383 in complex with benzoate, pyruvate and glutamine
Authors	:	Li, Q.A.; Mavrodi, D.V.; Thomashow, L.S.; Roessle, M.; Blankenfeldt, W.
Deposited on	:	2011-03-22
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

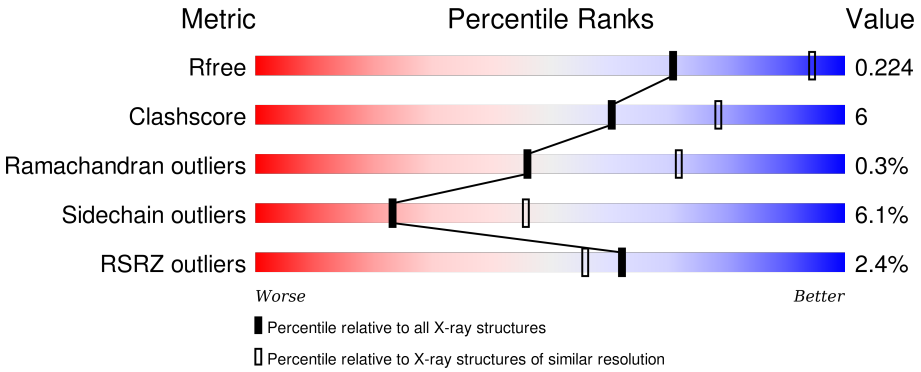
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 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 <=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% 10% • 5%
1	B	645	2% 80% 14% • •

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 6 unique types of molecules in this entry. The entry contains 9572 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	612	Total	C	N	O	S	0	2	0
			4595	2887	822	863	23			
1	B	622	Total	C	N	O	S	0	1	0
			4692	2937	845	888	22			

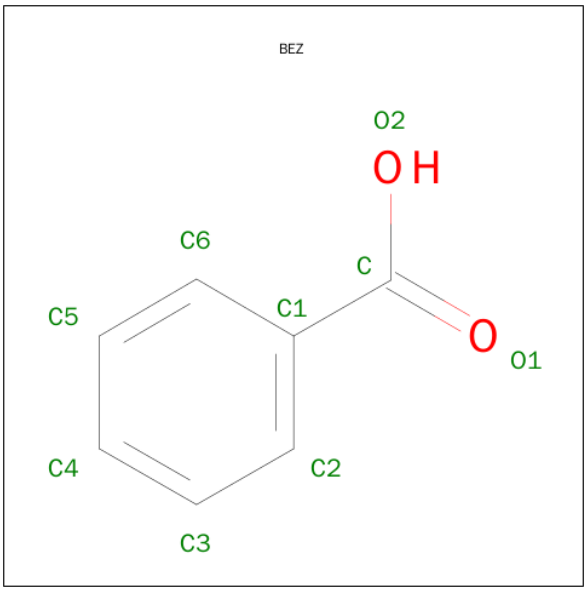
There are 4 discrepancies between the modelled and reference sequences:

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).

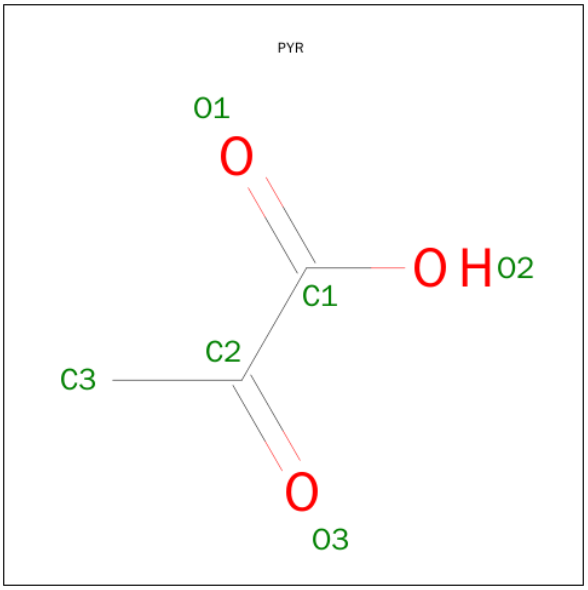
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



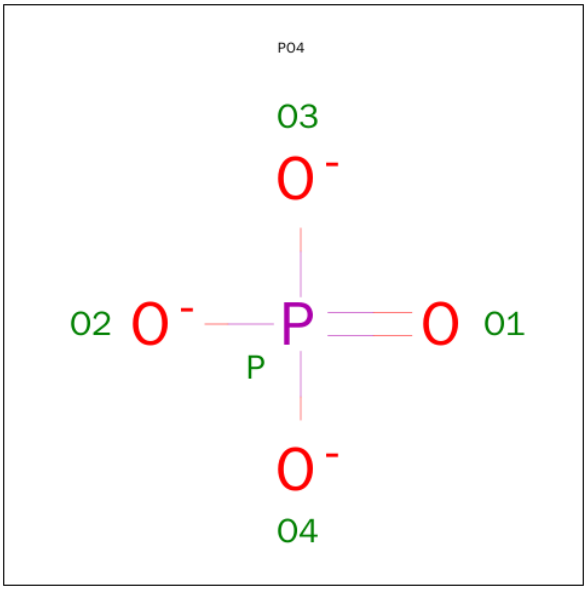
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0

- 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 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

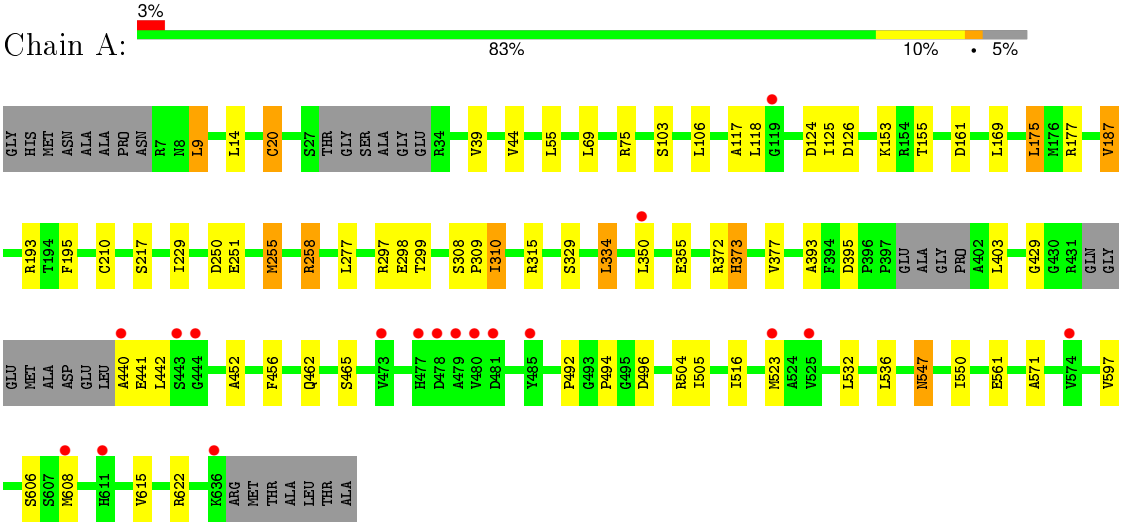
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	133	Total O 133 133	0	0
6	B	110	Total O 110 110	0	0

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 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 (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.

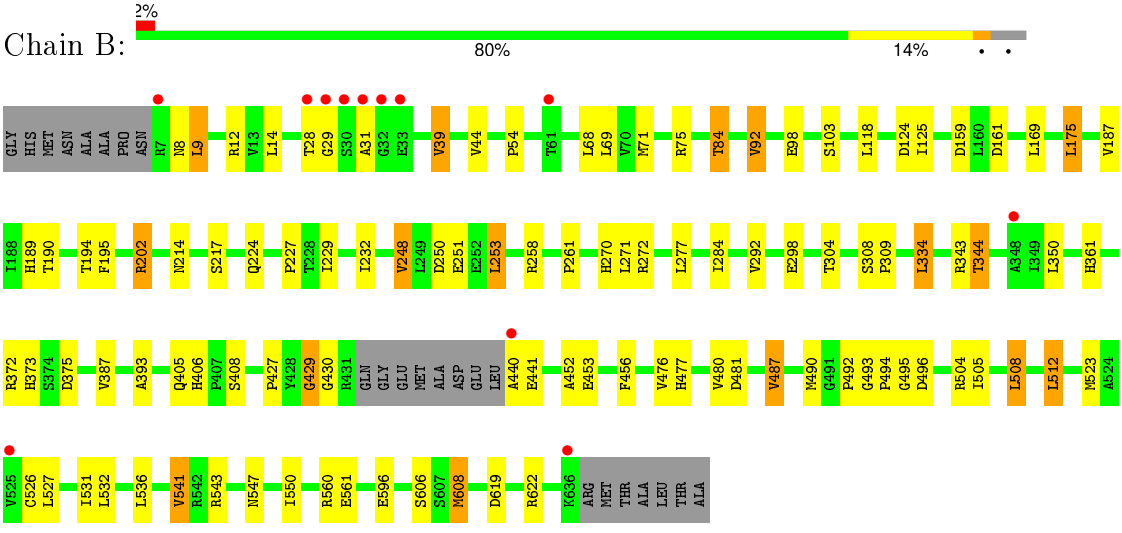
- Molecule 1: Anthranilate/para-aminobenzoate synthases component I

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	258.17Å 97.79Å 53.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 2.60 29.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.66-2.60) 99.8 (29.66-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.47 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.163 , 0.225 0.166 , 0.224	Depositor DCC
R_{free} test set	2227 reflections (5.46%)	DCC
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 43043 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9572	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BEZ, PO4, MG, 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	0.75	1/4677 (0.0%)	0.82	3/6360 (0.0%)
1	B	0.73	1/4774 (0.0%)	0.85	5/6490 (0.1%)
All	All	0.74	2/9451 (0.0%)	0.83	8/12850 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	CYS	CB-SG	-6.75	1.70	1.82
1	B	272	ARG	CG-CD	-5.47	1.38	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	487	VAL	CB-CA-C	-6.78	98.51	111.40
1	B	429	GLY	N-CA-C	6.57	129.53	113.10
1	B	272	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	B	272	ARG	CA-CB-CG	-6.17	99.83	113.40
1	A	258	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	541	VAL	CB-CA-C	-5.70	100.58	111.40
1	A	297	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	126	ASP	CB-CG-OD2	5.06	122.86	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	4595	0	4462	47	0
1	B	4692	0	4558	67	0
2	A	1	0	0	0	0
2	B	1	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	0	0
6	A	133	0	0	0	0
6	B	110	0	0	7	0
All	All	9572	0	9036	102	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 6.

All (102) 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:9:LEU:HD13	1:B:39:VAL:HG22	1.45	0.98
1:A:452:ALA:HB3	1:A:492:PRO:O	1.73	0.89
1:A:310:ILE:O	1:A:310:ILE:HD12	1.78	0.81
1:B:292:VAL:HG11	1:B:343:ARG:HD2	1.64	0.80
1:B:608:MET:HE1	6:B:654:HOH:O	1.79	0.80
1:A:9:LEU:HD13	1:A:39:VAL:HG12	1.64	0.79
1:B:344:THR:HG23	6:B:657:HOH:O	1.82	0.78
1:A:175:LEU:HD13	1:A:393:ALA:CB	2.17	0.75
1:A:403:LEU:HD13	1:B:232:ILE:HG13	1.71	0.73
1:A:210[B]:CYS:SG	6:B:660:HOH:O	2.46	0.73
1:B:292:VAL:HG13	1:B:343:ARG:HG2	1.72	0.72
1:B:512:LEU:HD23	1:B:531:ILE:HG22	1.73	0.70
1:B:75:ARG:HA	1:B:84:THR:HG21	1.74	0.69
1:B:277:LEU:HD12	1:B:277:LEU:C	2.13	0.69
1:B:253:LEU:HD13	1:B:284:ILE:HD13	1.75	0.67
1:B:292:VAL:HG11	1:B:343:ARG:CD	2.26	0.64
1:A:175:LEU:HD13	1:A:393:ALA:HB2	1.80	0.63
1:B:248:VAL:HG11	1:B:304:THR:HG22	1.79	0.63
1:A:277:LEU:C	1:A:277:LEU:HD12	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:HD22	1:B:229:ILE:HD13	1.80	0.62
1:B:495:GLY:O	1:B:526:CYG:N1	2.33	0.62
1:B:543:ARG:NH1	1:B:596:GLU:OE2	2.33	0.61
1:B:440:ALA:N	1:B:441:GLU:HA	2.15	0.60
1:B:69:LEU:HD13	1:B:334:LEU:HD13	1.83	0.60
1:B:452:ALA:HB3	1:B:492:PRO:O	2.02	0.59
1:B:344:THR:CG2	6:B:657:HOH:O	2.45	0.58
1:A:547:ASN:ND2	1:A:550:ILE:HG21	2.18	0.58
1:B:292:VAL:CG1	1:B:343:ARG:HG2	2.33	0.58
1:B:406:HIS:CD2	1:B:408:SER:OG	2.56	0.58
1:A:523:MET:HA	1:A:606:SER:O	2.04	0.58
1:A:258:ARG:NH2	1:A:298:GLU:OE1	2.36	0.58
1:B:248:VAL:CG1	1:B:304:THR:HG22	2.33	0.58
1:B:54:PRO:HD2	1:B:68:LEU:HD11	1.87	0.57
1:A:403:LEU:CD2	1:B:229:ILE:HD13	2.35	0.56
1:B:490:MET:HG3	1:B:512:LEU:CD1	2.36	0.56
1:B:175:LEU:HD13	1:B:393:ALA:HB2	1.86	0.56
1:B:480:VAL:HG12	1:B:481:ASP:N	2.21	0.56
1:A:229:ILE:HD11	1:B:406:HIS:CG	2.41	0.55
1:A:403:LEU:HD11	1:B:227:PRO:HB2	1.88	0.55
1:B:406:HIS:HD2	1:B:408:SER:OG	1.90	0.54
1:B:427:PRO:O	1:B:430:GLY:HA3	2.07	0.54
1:B:523:MET:HA	1:B:606:SER:O	2.07	0.54
1:B:258:ARG:NH2	1:B:298:GLU:OE1	2.41	0.53
1:A:153:LYS:HE3	1:A:155:THR:OG1	2.09	0.53
1:B:608:MET:CE	6:B:654:HOH:O	2.44	0.53
1:A:255:MET:HE3	1:A:299:THR:HB	1.90	0.52
1:A:20:CYS:SG	1:A:44:VAL:HG22	2.50	0.52
1:B:12:ARG:NH2	1:B:98:GLU:OE2	2.42	0.52
1:B:277:LEU:O	1:B:277:LEU:HD12	2.09	0.52
1:A:308:SER:HA	1:A:309:PRO:C	2.30	0.52
1:A:310:ILE:HD12	1:A:310:ILE:C	2.29	0.51
1:B:202:ARG:HD2	6:B:689:HOH:O	2.11	0.51
1:A:403:LEU:HD13	1:B:232:ILE:CG1	2.40	0.50
1:A:615:VAL:HG22	1:B:250:ASP:OD1	2.11	0.50
1:A:9:LEU:HD13	1:A:39:VAL:CG1	2.36	0.50
1:A:547:ASN:HD22	1:A:550:ILE:HG21	1.76	0.50
1:B:308:SER:HA	1:B:309:PRO:C	2.31	0.50
1:A:193:ARG:HH11	1:A:355:GLU:HB3	1.77	0.50
1:B:476:VAL:HG23	1:B:477:HIS:CD2	2.47	0.49
1:A:251:GLU:CD	1:A:308:SER:CB	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ASP:O	1:B:505:ILE:HD13	2.13	0.49
1:A:315:ARG:NH2	1:B:453:GLU:OE1	2.45	0.48
1:B:292:VAL:CG1	1:B:343:ARG:CG	2.91	0.48
1:A:255:MET:CE	1:A:299:THR:HB	2.44	0.48
1:A:516:ILE:HD11	1:A:532:LEU:CD1	2.44	0.48
1:B:561:GLU:OE2	1:B:622:ARG:NH2	2.46	0.48
1:B:251:GLU:CD	1:B:308:SER:CB	2.82	0.48
1:B:277:LEU:CD1	1:B:277:LEU:C	2.82	0.48
1:B:71:MET:HB2	1:B:92:VAL:HG13	1.96	0.47
1:B:619:ASP:OD2	1:B:622:ARG:NH1	2.47	0.47
1:B:512:LEU:HD23	1:B:531:ILE:CG2	2.44	0.46
1:B:44:VAL:HG21	1:B:190:THR:O	2.15	0.46
1:A:187:VAL:HA	1:A:195:PHE:O	2.16	0.46
1:B:189:HIS:HD2	1:B:194:THR:OG1	1.99	0.46
1:A:571:ALA:HB3	1:A:597:VAL:HB	1.99	0.45
1:B:532:LEU:O	1:B:536:LEU:HG	2.18	0.44
1:B:270:HIS:HE1	6:B:731:HOH:O	1.99	0.44
1:A:175:LEU:CD1	1:A:393:ALA:HB2	2.45	0.44
1:B:494:PRO:O	1:B:504:ARG:NH2	2.37	0.44
1:A:462:GLN:NE2	1:B:261:PRO:O	2.51	0.44
1:A:496:ASP:O	1:A:505:ILE:HD13	2.17	0.44
1:A:494:PRO:O	1:A:504:ARG:NH2	2.39	0.44
1:A:532:LEU:O	1:A:536:LEU:HG	2.17	0.44
1:A:561:GLU:OE2	1:A:622:ARG:NH2	2.50	0.43
1:B:429:GLY:N	1:B:430:GLY:HA3	2.33	0.43
1:B:187:VAL:HA	1:B:195:PHE:O	2.18	0.43
1:A:69:LEU:HD13	1:A:334:LEU:HD13	2.00	0.43
1:B:493:GLY:O	1:B:527:LEU:HD22	2.19	0.43
1:B:440:ALA:N	1:B:441:GLU:CA	2.82	0.42
1:A:372:ARG:NH2	1:B:550:ILE:HD12	2.35	0.42
1:A:55:LEU:HA	1:A:55:LEU:HD23	1.84	0.42
1:A:117:ALA:HA	1:A:395:ASP:OD1	2.20	0.41
1:A:373:HIS:ND1	1:A:373:HIS:N	2.68	0.41
1:B:476:VAL:HG11	1:B:508:LEU:CD1	2.50	0.41
1:A:440:ALA:O	1:A:441:GLU:HB2	2.20	0.41
1:A:547:ASN:HD22	1:A:547:ASN:HA	1.62	0.41
1:B:124:ASP:OD1	1:B:125:ILE:N	2.52	0.41
1:B:202:ARG:HD3	1:B:214:ASN:HB2	2.02	0.41
1:B:159:ASP:OD1	1:B:361:HIS:HD2	2.03	0.41
1:A:124:ASP:OD1	1:A:125:ILE:N	2.52	0.41
1:A:229:ILE:HD11	1:B:406:HIS:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ILE:HD12	1:B:372:ARG:NH2	2.37	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	605/645 (94%)	588 (97%)	16 (3%)	1 (0%)	52 77
1	B	618/645 (96%)	598 (97%)	17 (3%)	3 (0%)	34 60
All	All	1223/1290 (95%)	1186 (97%)	33 (3%)	4 (0%)	46 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	THR
1	B	29	GLY
1	A	429	GLY
1	B	31	ALA

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	462/506 (91%)	437 (95%)	25 (5%)	27 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	473/506 (94%)	441 (93%)	32 (7%)	20 39
All	All	935/1012 (92%)	878 (94%)	57 (6%)	23 46

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	14	LEU
1	A	75	ARG
1	A	103	SER
1	A	106	LEU
1	A	118	LEU
1	A	161	ASP
1	A	169	LEU
1	A	175	LEU
1	A	177	ARG
1	A	187	VAL
1	A	217	SER
1	A	250	ASP
1	A	255	MET
1	A	310	ILE
1	A	329	SER
1	A	334	LEU
1	A	350	LEU
1	A	373	HIS
1	A	377	VAL
1	A	442	LEU
1	A	456	PHE
1	A	465	SER
1	A	547	ASN
1	A	608	MET
1	B	8	ASN
1	B	9	LEU
1	B	14	LEU
1	B	39	VAL
1	B	84	THR
1	B	92	VAL
1	B	103	SER
1	B	118	LEU
1	B	161	ASP
1	B	169	LEU
1	B	175	LEU

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Mol	Chain	Res	Type
1	B	202	ARG
1	B	217	SER
1	B	224	GLN
1	B	248	VAL
1	B	253	LEU
1	B	271	LEU
1	B	334	LEU
1	B	344	THR
1	B	350	LEU
1	B	373	HIS
1	B	375	ASP
1	B	387	VAL
1	B	405	GLN
1	B	456	PHE
1	B	487	VAL
1	B	508	LEU
1	B	512	LEU
1	B	541	VAL
1	B	547	ASN
1	B	560	ARG
1	B	608	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	189	HIS
1	A	392	ASN
1	A	410	GLN
1	A	462	GLN
1	A	547	ASN
1	B	17	GLN
1	B	189	HIS
1	B	361	HIS
1	B	406	HIS
1	B	462	GLN
1	B	477	HIS
1	B	547	ASN
1	B	572	GLN

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	10,14,15	1.82	4 (40%)	6,17,19	3.12	3 (50%)
1	CYG	B	526	1	10,14,15	2.13	4 (40%)	6,17,19	2.95	4 (66%)

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	-	0/10/16/18	0/0/0/0
1	CYG	B	526	1	-	0/10/16/18	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	526	CYG	CB-SG	2.02	1.84	1.81
1	A	526	CYG	CD1-SG	2.54	1.81	1.76
1	B	526	CYG	CD1-SG	2.77	1.82	1.76
1	A	526	CYG	OE2-CD1	2.79	1.25	1.21
1	B	526	CYG	OE2-CD1	3.07	1.25	1.21
1	B	526	CYG	CB-SG	3.30	1.86	1.81
1	A	526	CYG	CG1-CD1	3.58	1.54	1.50
1	B	526	CYG	CG1-CD1	3.94	1.55	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	CYG	OE2-CD1-CG1	-5.55	120.12	123.94
1	B	526	CYG	OE2-CD1-CG1	-5.30	120.29	123.94
1	B	526	CYG	CB1-CG1-CD1	-2.65	109.21	113.12
1	B	526	CYG	O-C-CA	-2.22	119.69	125.49
1	A	526	CYG	O-C-CA	-2.02	120.22	125.49
1	B	526	CYG	CG1-CD1-SG	2.60	115.69	113.36
1	A	526	CYG	CG1-CD1-SG	4.53	117.43	113.36

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
1	B	526	CYG	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 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	0.51	0	8,11,11	0.51	0
4	PYR	A	702	-	2,5,5	0.07	0	2,6,6	0.87	0
5	PO4	A	900	-	4,4,4	0.73	0	6,6,6	0.29	0
3	BEZ	B	701	2	6,9,9	0.70	0	8,11,11	0.37	0
4	PYR	B	702	-	2,5,5	0.56	0	2,6,6	1.18	0
5	PO4	B	900	-	4,4,4	0.19	0	6,6,6	0.27	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

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

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^{th} 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	611/645 (94%)	-0.19	18 (2%)	55	48	26, 50, 80, 127	0
1	B	621/645 (96%)	-0.17	12 (1%)	70	64	32, 50, 78, 121	0
All	All	1232/1290 (95%)	-0.18	30 (2%)	62	56	26, 50, 79, 127	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	ALA	6.2
1	B	440	ALA	5.1
1	B	32	GLY	4.7
1	B	30	SER	4.6
1	A	480	VAL	4.3
1	B	29	GLY	4.0
1	B	33	GLU	3.7
1	A	481	ASP	3.6
1	B	31	ALA	3.5
1	A	574	VAL	3.0
1	A	477	HIS	2.9
1	A	636	LYS	2.9
1	A	611	HIS	2.9
1	A	608	MET	2.9
1	B	28	THR	2.8
1	B	7	ARG	2.8
1	A	444	GLY	2.8
1	B	61	THR	2.7
1	B	525	VAL	2.7
1	A	473	VAL	2.7
1	A	525	VAL	2.6
1	A	485	TYR	2.5
1	B	348	ALA	2.5
1	A	478	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	443	SER	2.4
1	A	119	GLY	2.3
1	B	636	LYS	2.3
1	A	350	LEU	2.3
1	A	523	MET	2.3
1	A	479	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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	0.95	0.19	-	32,39,45,47	0
1	CYG	A	526	15/16	0.94	0.24	-	47,67,80,83	0

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^{th} 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	A	900	5/5	0.87	0.35	7.60	20,22,22,23	5
5	PO4	B	900	5/5	0.90	0.34	4.66	71,96,103,106	0
4	PYR	A	702	6/6	0.98	0.30	1.96	38,42,44,49	0
3	BEZ	A	701	9/9	0.99	0.26	1.29	33,35,37,38	0
4	PYR	B	702	6/6	0.95	0.24	0.94	43,52,58,59	0
3	BEZ	B	701	9/9	0.98	0.20	0.33	38,40,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	700	1/1	0.98	0.16	-0.00	45,45,45,45	0
2	MG	B	700	1/1	0.99	0.13	-0.30	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.