W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2014 – 06:07 AM GMT

PDB ID	:	3R5B
Title	:	Pseudomonas aeruginosa DapD (PA3666) in complex with L-2-aminopimelate
Authors	:	Sandalova, T.; Schnell, R.; Schneider, G.
Deposited on	:	2011-03-18
Resolution	:	2.51 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.51 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		5.1%
RSRZ outliers		0.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
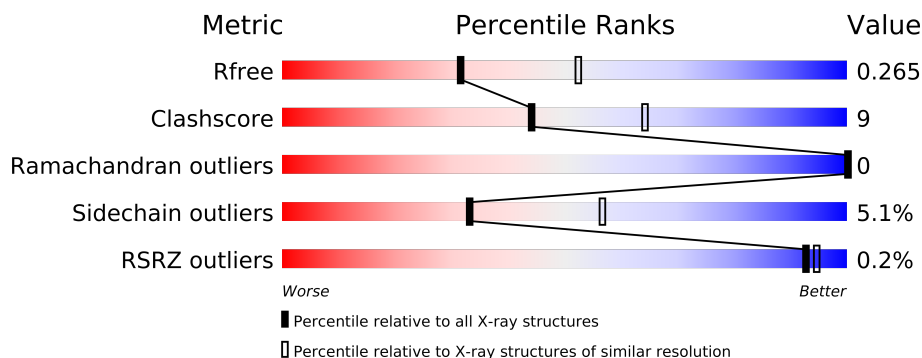
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	
1	F	347	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NPI	A	381	-	X
2	NPI	E	381	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14397 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TetrahydrodipicolinateN-succinyletransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2364	1506	406	445	7			
1	B	318	Total	C	N	O	S	0	0	0
			2342	1492	403	440	7			
1	C	321	Total	C	N	O	S	0	0	0
			2367	1506	407	447	7			
1	D	321	Total	C	N	O	S	0	0	0
			2364	1506	406	445	7			
1	E	310	Total	C	N	O	S	0	0	0
			2277	1455	386	429	7			
1	F	321	Total	C	N	O	S	0	0	0
			2367	1506	407	447	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
A	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
A	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
B	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
B	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
B	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
C	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
C	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
C	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
D	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
D	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
D	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
E	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
E	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2
E	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2
F	-2	GLY	-	EXPRESSION TAG	UNP Q9Z9H2
F	-1	SER	-	EXPRESSION TAG	UNP Q9Z9H2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	EXPRESSION TAG	UNP Q9Z9H2

- Molecule 2 is (2S)-2-AMINOHEPTANEDIOICACID (three-letter code: NPI) (formula: $C_7H_{13}NO_4$).
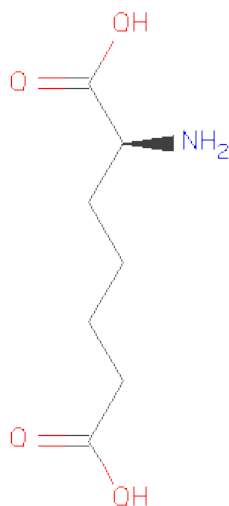
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 12	C 7	N 1	O 4	0	0
2	C	1	Total 12	C 7	N 1	O 4	0	0
2	D	1	Total 12	C 7	N 1	O 4	0	0
2	E	1	Total 12	C 7	N 1	O 4	0	0
2	E	1	Total 12	C 7	N 1	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total 43	O 43	0	0
3	B	53	Total 53	O 53	0	0
3	C	44	Total 44	O 44	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	36	Total 36	O 36	0	0
3	E	47	Total 47	O 47	0	0
3	F	33	Total 33	O 33	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 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.
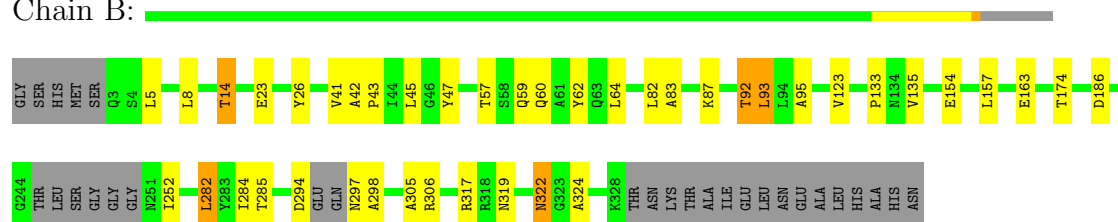
- Molecule 1: TetrahydrodipicolinateN-succinyletransferase
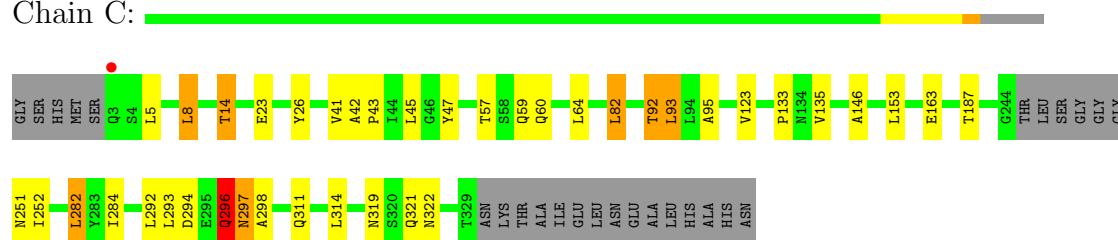
Chain A:
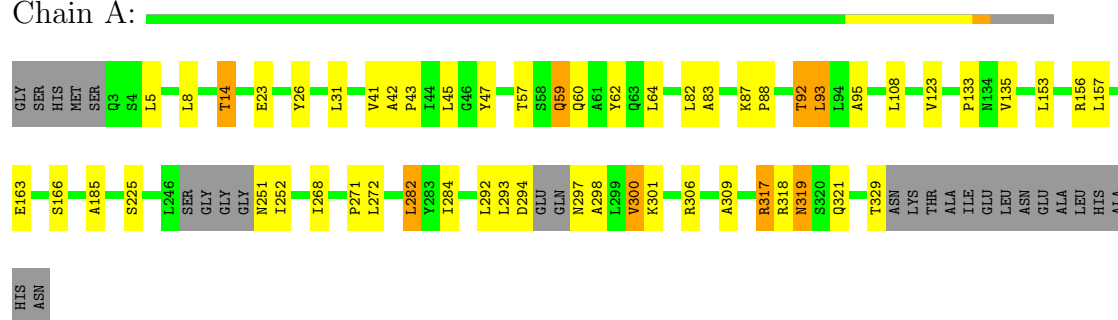
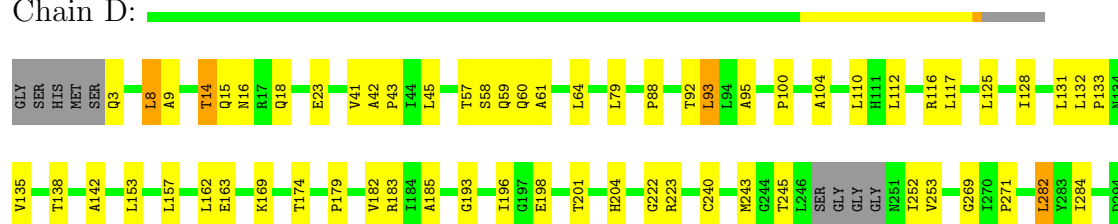- Molecule 1: TetrahydrodipicolinateN-succinyletransferase

Chain B:

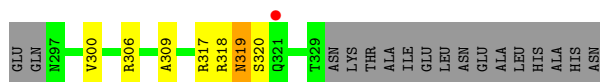- Molecule 1: TetrahydrodipicolinateN-succinyletransferase

Chain C:

- Molecule 1: TetrahydrodipicolinateN-succinyletransferase

Chain D:

GLU GLN N297 V300 R306 A309 R317 R318 N319 S320 Q321 T329 ASN LYS THR ALA ILE GLU LEU ASN GLU ALA LEU HIS ALA HIS ASN

• Molecule 1: TetrahydrodipicolinateN-succinyletransferase

Chain E:

GLY SER HIS MET SER Q3 S4 L5 L8 A9 T14 Q15 N16 R17 Q18 E23 V24 F25 V41 A42 P43 Y47 T57 S58 Q59 Q60 A61 Y62 A65 D66 G70 S76 R81 L82 A83 E84 P88 L89 T92 L93 L94 A95 P100 A104 L113

V123 L131 L132 P133 N134 V135 V143 D144 E154 E163 V164 F165 Y176 V182 G193 A194 Y195 I196 N209 A212 G213 S241 T242 M243 GLY THR LEU SER GLY GLY GLY N251 I252 I268 G269 I270 L282 Y283 I284 T285 D294 GLU GLN N297 A298

V302 A305 R306 Q311 L315 PHE ARG ARG ASN SER GLN ASN GLY A324 T329 ASN LYS THR ALA ILE GLU LEU ASN GLU ALA LEU HIS ALA HIS ASN

• Molecule 1: TetrahydrodipicolinateN-succinyletransferase

Chain F:

GLY SER HIS MET SER Q3 S4 L5 L8 T14 E23 L28 V41 A42 P43 T44 L45 T57 S58 Q59 Q60 A61 Y62 Q63 L64 A65 L78 L79 A83 E84 S85 Q86 K87 P88 T92 L93 L94 A95 A98 A104 E105 L108 K109 R116 P120

V135 T138 V143 E147 L153 E154 L157 E163 V164 F165 T174 V177 V178 P179 A180 G181 V182 R189 G197 G206 T214 F229 V230 G244 THR LEU SER GLY GLY GLY N251 I252 V253 V254 L272 N276 L282 Y283 I284 L293 D294 E295

Q296 N297 A298 L299 V302 N319 S320 Q321 N322 K328 T329 ASN LYS THR ALA ILE GLU LEU ASN GLU ALA LEU HIS ALA HIS ASN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.04Å 102.00Å 134.90Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	36.88 – 2.51 36.88 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.9 (36.88-2.51) 97.3 (36.88-2.51)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.250 , 0.276 0.243 , 0.265	Depositor DCC
R_{free} test set	3763 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 7.1	EDS
Estimated twinning fraction	0.545 for H, K, L 0.455 for H, -K, -L 0.326 for h,-k,-l	Xtriage
Reported twinning fraction	0.545 for H, K, L 0.455 for H, -K, -L	Depositor
L-test for twinning	$< |L| > = 0.38, < L^2 > = 0.20$	Xtriage
Outliers	0 of 74974 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	14397	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NPI

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	0.51	0/2400	0.63	1/3257 (0.0%)
1	B	0.50	0/2378	0.61	0/3226
1	C	0.50	0/2404	0.66	3/3263 (0.1%)
1	D	0.54	0/2400	0.66	0/3257
1	E	0.54	1/2311 (0.0%)	0.67	0/3137
1	F	0.52	0/2404	0.66	0/3263
All	All	0.52	1/14297 (0.0%)	0.65	4/19403 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	163	GLU	CG-CD	5.69	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	GLN	CB-CA-C	-10.44	89.52	110.40
1	C	296	GLN	N-CA-C	8.64	134.34	111.00
1	C	297	ASN	N-CA-CB	6.55	122.39	110.60
1	A	300	VAL	CG1-CB-CG2	6.26	120.92	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts (i)

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2364	0	2420	39	0
1	B	2342	0	2395	32	0
1	C	2367	0	2417	32	0
1	D	2364	0	2420	46	0
1	E	2277	0	2335	48	0
1	F	2367	0	2417	56	0
2	A	12	0	11	1	0
2	C	12	0	11	1	0
2	D	12	0	11	0	0
2	E	24	0	22	0	0
3	A	43	0	0	3	0
3	B	53	0	0	4	0
3	C	44	0	0	2	0
3	D	36	0	0	2	0
3	E	47	0	0	1	0
3	F	33	0	0	1	0
All	All	14397	0	14459	245	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 245 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:296:GLN:O	1:C:296:GLN:HG3	1.49	1.10
1:D:182:VAL:HG11	1:D:196:ILE:HG21	1.46	0.95
1:D:3:GLN:HE22	1:D:95:ALA:HB1	1.37	0.90
1:C:296:GLN:O	1:C:296:GLN:CG	2.16	0.89
1:E:62:TYR:CE1	1:E:83:ALA:HB1	2.12	0.84

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	315/347 (91%)	310 (98%)	5 (2%)	0	100	100
1	B	312/347 (90%)	308 (99%)	4 (1%)	0	100	100
1	C	317/347 (91%)	313 (99%)	4 (1%)	0	100	100
1	D	315/347 (91%)	297 (94%)	18 (6%)	0	100	100
1	E	302/347 (87%)	291 (96%)	11 (4%)	0	100	100
1	F	317/347 (91%)	304 (96%)	13 (4%)	0	100	100
All	All	1878/2082 (90%)	1823 (97%)	55 (3%)	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	244/263 (93%)	231 (95%)	13 (5%)	32	54
1	B	241/263 (92%)	229 (95%)	12 (5%)	34	58
1	C	244/263 (93%)	234 (96%)	10 (4%)	41	67
1	D	244/263 (93%)	230 (94%)	14 (6%)	29	50
1	E	235/263 (89%)	220 (94%)	15 (6%)	25	43
1	F	244/263 (93%)	234 (96%)	10 (4%)	41	67
All	All	1452/1578 (92%)	1378 (95%)	74 (5%)	33	57

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	282	LEU
1	D	245	THR
1	F	153	LEU
1	C	296	GLN
1	D	93	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	319	ASN
1	D	52	GLN
1	F	276	ASN
1	D	15	GLN
1	D	60	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

5 ligands 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	#$|Z| > 2$
2	NPI	A	381	-	11,11,11	0.87	0	13,13,13	1.01	0
2	NPI	C	381	-	11,11,11	1.08	1 (9%)	13,13,13	0.93	1 (7%)
2	NPI	D	381	-	11,11,11	1.04	0	13,13,13	1.08	0
2	NPI	E	345	-	11,11,11	1.15	0	13,13,13	0.95	1 (7%)
2	NPI	E	381	-	11,11,11	1.07	0	13,13,13	1.07	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
2	NPI	A	381	-	-	0/11/11/11	0/0/0/0
2	NPI	C	381	-	-	0/11/11/11	0/0/0/0
2	NPI	D	381	-	-	0/11/11/11	0/0/0/0
2	NPI	E	345	-	-	0/11/11/11	0/0/0/0
2	NPI	E	381	-	-	0/11/11/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	381	NPI	C6-C7	2.34	1.56	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	345	NPI	C-CA-N	-2.24	105.66	109.36
2	C	381	NPI	C-CA-N	2.05	112.75	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7   Other polymers (i)

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(Å²)	Q<0.9
1	A	321/347 (92%)	-0.20	0	100	100	12, 17, 48, 68	0
1	B	318/347 (91%)	-0.24	0	100	100	11, 16, 43, 56	0
1	C	321/347 (92%)	-0.16	1 (0%)	91	93	12, 18, 46, 55	0
1	D	321/347 (92%)	-0.11	1 (0%)	91	93	12, 18, 50, 76	0
1	E	310/347 (89%)	-0.21	1 (0%)	91	93	11, 17, 44, 59	0
1	F	321/347 (92%)	-0.14	1 (0%)	91	93	13, 19, 50, 58	0
All	All	1912/2082 (91%)	-0.18	4 (0%)	93	94	11, 18, 48, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	321	GLN	3.2
1	F	302	VAL	2.1
1	E	302	VAL	2.0
1	C	3	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	NPI	E	381	12/12	0.17	2.90	2,2,5,5	0
2	NPI	A	381	12/12	0.17	2.04	7,8,10,10	0
2	NPI	C	381	12/12	0.16	1.32	6,11,20,22	0
2	NPI	E	345	12/12	0.15	0.82	8,16,19,20	0
2	NPI	D	381	12/12	0.15	0.24	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.