



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:25 AM GMT

PDB ID : 3EJX
Title : Crystal structure of diaminopimelate epimerase from *Arabidopsis thaliana* in complex with LL-AziDAP
Authors : Pillai, B.; Moorthie, V.A.; Cherney, M.M.; Vederas, J.C.; James, M.N.G.
Deposited on : 2008-09-18
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

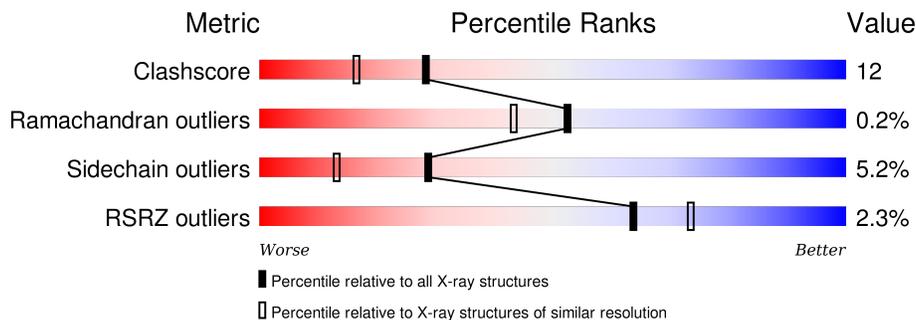
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	
1	F	317	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15115 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 Diaminopimelate epimerase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2169	1363	377	413	16	0	0	0
1	B	288	2179	1369	380	414	16	0	0	0
1	C	287	2169	1363	377	413	16	0	0	0
1	D	301	2273	1430	393	434	16	6	0	0
1	E	287	2169	1363	377	413	16	0	0	0
1	F	301	2273	1430	393	434	16	6	0	0

There are 36 discrepancies between the modelled and reference sequences:

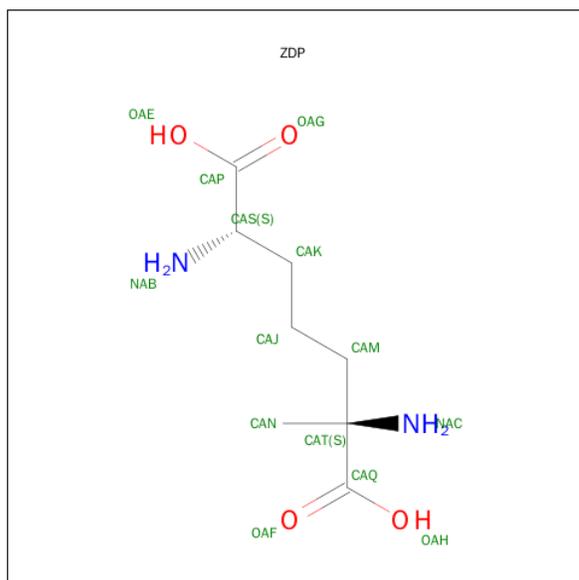
Chain	Residue	Modelled	Actual	Comment	Reference
A	312	HIS	-	EXPRESSION TAG	UNP Q9LFG2
A	313	HIS	-	EXPRESSION TAG	UNP Q9LFG2
A	314	HIS	-	EXPRESSION TAG	UNP Q9LFG2
A	315	HIS	-	EXPRESSION TAG	UNP Q9LFG2
A	316	HIS	-	EXPRESSION TAG	UNP Q9LFG2
A	317	HIS	-	EXPRESSION TAG	UNP Q9LFG2
B	312	HIS	-	EXPRESSION TAG	UNP Q9LFG2
B	313	HIS	-	EXPRESSION TAG	UNP Q9LFG2
B	314	HIS	-	EXPRESSION TAG	UNP Q9LFG2
B	315	HIS	-	EXPRESSION TAG	UNP Q9LFG2
B	316	HIS	-	EXPRESSION TAG	UNP Q9LFG2
B	317	HIS	-	EXPRESSION TAG	UNP Q9LFG2
C	312	HIS	-	EXPRESSION TAG	UNP Q9LFG2
C	313	HIS	-	EXPRESSION TAG	UNP Q9LFG2
C	314	HIS	-	EXPRESSION TAG	UNP Q9LFG2
C	315	HIS	-	EXPRESSION TAG	UNP Q9LFG2
C	316	HIS	-	EXPRESSION TAG	UNP Q9LFG2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	317	HIS	-	EXPRESSION TAG	UNP Q9LFG2
D	312	HIS	-	EXPRESSION TAG	UNP Q9LFG2
D	313	HIS	-	EXPRESSION TAG	UNP Q9LFG2
D	314	HIS	-	EXPRESSION TAG	UNP Q9LFG2
D	315	HIS	-	EXPRESSION TAG	UNP Q9LFG2
D	316	HIS	-	EXPRESSION TAG	UNP Q9LFG2
D	317	HIS	-	EXPRESSION TAG	UNP Q9LFG2
E	312	HIS	-	EXPRESSION TAG	UNP Q9LFG2
E	313	HIS	-	EXPRESSION TAG	UNP Q9LFG2
E	314	HIS	-	EXPRESSION TAG	UNP Q9LFG2
E	315	HIS	-	EXPRESSION TAG	UNP Q9LFG2
E	316	HIS	-	EXPRESSION TAG	UNP Q9LFG2
E	317	HIS	-	EXPRESSION TAG	UNP Q9LFG2
F	312	HIS	-	EXPRESSION TAG	UNP Q9LFG2
F	313	HIS	-	EXPRESSION TAG	UNP Q9LFG2
F	314	HIS	-	EXPRESSION TAG	UNP Q9LFG2
F	315	HIS	-	EXPRESSION TAG	UNP Q9LFG2
F	316	HIS	-	EXPRESSION TAG	UNP Q9LFG2
F	317	HIS	-	EXPRESSION TAG	UNP Q9LFG2

- Molecule 2 is (2S,6S)-2,6-DIAMINO-2-METHYLHEPTANEDIOIC ACID (three-letter code: ZDP) (formula: C₈H₁₆N₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	N	O	0	0
			14	8	2	4		

Continued on next page...

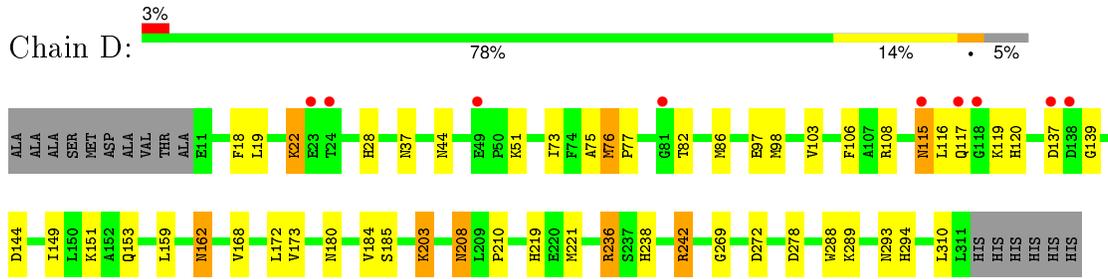
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	2	4		
2	C	1	Total	C	N	O	0	0
			14	8	2	4		
2	D	1	Total	C	N	O	0	0
			14	8	2	4		
2	E	1	Total	C	N	O	0	0
			14	8	2	4		
2	F	1	Total	C	N	O	0	0
			14	8	2	4		

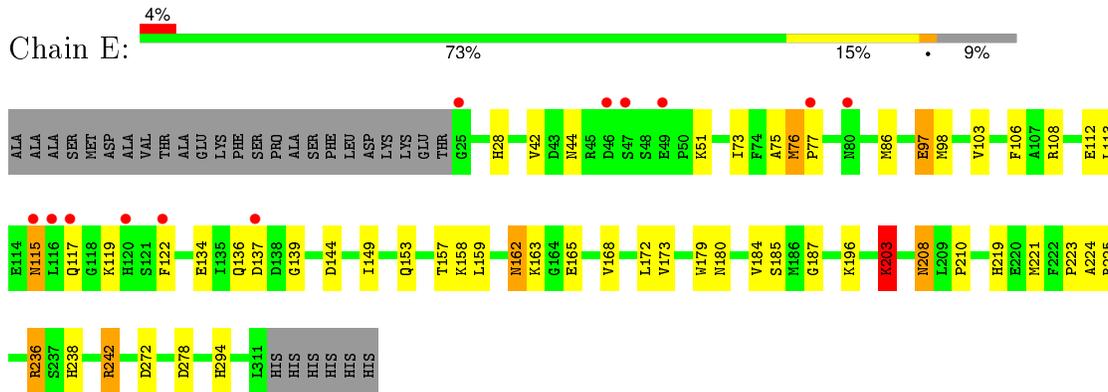
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	339	Total	O	0	0
			339	339		
3	B	338	Total	O	0	0
			338	338		
3	C	317	Total	O	0	0
			317	317		
3	D	280	Total	O	0	0
			280	280		
3	E	293	Total	O	0	0
			293	293		
3	F	232	Total	O	0	0
			232	232		

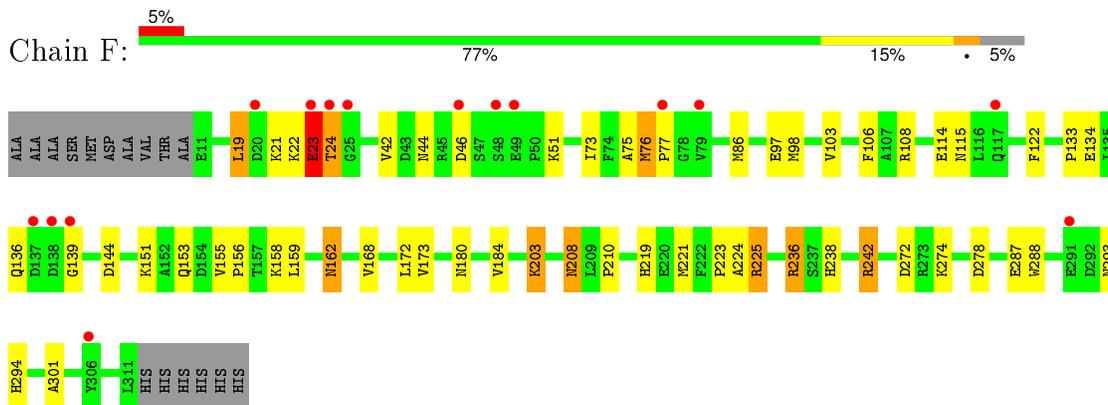
- Molecule 1: Diaminopimelate epimerase, chloroplastic



- Molecule 1: Diaminopimelate epimerase, chloroplastic



- Molecule 1: Diaminopimelate epimerase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.54Å 136.44Å 102.57Å 90.00° 119.54° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 42.14 – 1.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.95) 97.7 (42.14-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.95Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.208 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.8	Xtrriage
Anisotropy	0.250	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.1	EDS
Estimated twinning fraction	0.001 for -h-l,k,h 0.001 for l,k,-h-l 0.014 for h,-k,-h-l 0.013 for -h-l,-k,l 0.014 for l,-k,h	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 175374 reflections	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15115	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZDP

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	0.53	0/2214	0.78	4/2998 (0.1%)
1	B	0.51	0/2225	0.74	3/3013 (0.1%)
1	C	0.52	0/2214	0.76	4/2998 (0.1%)
1	D	0.54	2/2321 (0.1%)	0.76	4/3141 (0.1%)
1	E	0.49	0/2214	0.74	3/2998 (0.1%)
1	F	0.45	0/2321	0.78	5/3141 (0.2%)
All	All	0.51	2/13509 (0.0%)	0.76	23/18289 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	GLU	CD-OE1	-8.59	1.16	1.25
1	D	97	GLU	CD-OE2	-6.28	1.18	1.25

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	225	ARG	NE-CZ-NH1	-11.67	114.47	120.30
1	F	225	ARG	NE-CZ-NH2	11.11	125.85	120.30
1	A	242	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	D	97	GLU	OE1-CD-OE2	-9.33	112.11	123.30
1	A	242	ARG	NE-CZ-NH1	8.05	124.33	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2169	0	2121	50	0
1	B	2179	0	2128	53	0
1	C	2169	0	2121	50	0
1	D	2273	0	2217	58	0
1	E	2169	0	2121	48	0
1	F	2273	0	2217	53	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	339	0	0	7	0
3	B	338	0	0	6	0
3	C	317	0	0	7	0
3	D	280	0	0	7	0
3	E	293	0	0	3	0
3	F	232	0	0	4	0
All	All	15115	0	13003	305	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 12.

The worst 5 of 305 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:E:162:ASN:HD21	1:E:168:VAL:H	1.09	0.99
1:E:157:THR:HG22	1:E:159:LEU:H	1.31	0.96
1:A:162:ASN:HD21	1:A:168:VAL:H	1.12	0.95
1:F:162:ASN:HD21	1:F:168:VAL:H	1.07	0.94
1:C:162:ASN:HD21	1:C:168:VAL:H	1.08	0.92

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	285/317 (90%)	279 (98%)	6 (2%)	0	100	100
1	B	286/317 (90%)	279 (98%)	7 (2%)	0	100	100
1	C	285/317 (90%)	277 (97%)	8 (3%)	0	100	100
1	D	299/317 (94%)	287 (96%)	11 (4%)	1 (0%)	46	35
1	E	285/317 (90%)	281 (99%)	4 (1%)	0	100	100
1	F	299/317 (94%)	290 (97%)	6 (2%)	3 (1%)	19	8
All	All	1739/1902 (91%)	1693 (97%)	42 (2%)	4 (0%)	52	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	23	GLU
1	F	24	THR
1	D	82	THR
1	F	21	LYS

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	231/255 (91%)	219 (95%)	12 (5%)	29	13
1	B	232/255 (91%)	221 (95%)	11 (5%)	32	16
1	C	231/255 (91%)	218 (94%)	13 (6%)	26	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	242/255 (95%)	231 (96%)	11 (4%)	34	18
1	E	231/255 (91%)	217 (94%)	14 (6%)	23	9
1	F	242/255 (95%)	230 (95%)	12 (5%)	30	14
All	All	1409/1530 (92%)	1336 (95%)	73 (5%)	29	13

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	208	ASN
1	D	115	ASN
1	F	162	ASN
1	D	37	ASN
1	D	172	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	219	HIS
1	D	120	HIS
1	F	208	ASN
1	C	238	HIS
1	D	44	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	ZDP	A	500	-	5,13,13	0.68	0	3,18,18	0.33	0
2	ZDP	B	500	-	5,13,13	0.62	0	3,18,18	0.23	0
2	ZDP	C	500	-	5,13,13	0.57	0	3,18,18	0.38	0
2	ZDP	D	500	-	5,13,13	0.60	0	3,18,18	0.07	0
2	ZDP	E	500	-	5,13,13	0.55	0	3,18,18	0.25	0
2	ZDP	F	500	-	5,13,13	0.81	0	3,18,18	0.12	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	ZDP	A	500	-	-	0/7/17/17	0/0/0/0
2	ZDP	B	500	-	-	0/7/17/17	0/0/0/0
2	ZDP	C	500	-	-	0/7/17/17	0/0/0/0
2	ZDP	D	500	-	-	0/7/17/17	0/0/0/0
2	ZDP	E	500	-	-	0/7/17/17	0/0/0/0
2	ZDP	F	500	-	-	0/7/17/17	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	287/317 (90%)	0.01	1 (0%) 94 96	14, 19, 33, 42	0
1	B	288/317 (90%)	-0.12	2 (0%) 89 93	14, 21, 35, 48	0
1	C	287/317 (90%)	-0.23	2 (0%) 89 93	15, 21, 36, 46	0
1	D	301/317 (94%)	-0.03	9 (2%) 54 64	16, 24, 46, 62	2 (0%)
1	E	287/317 (90%)	0.06	12 (4%) 40 51	16, 23, 44, 50	0
1	F	301/317 (94%)	0.15	15 (4%) 32 44	17, 28, 54, 64	2 (0%)
All	All	1751/1902 (92%)	-0.03	41 (2%) 64 73	14, 23, 42, 64	4 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	79	VAL	4.8
1	F	46	ASP	4.7
1	F	137	ASP	4.3
1	F	23	GLU	3.8
1	D	23	GLU	3.7

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, 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
2	ZDP	A	500	14/14	0.97	0.16	0.93	12,15,16,17	0
2	ZDP	C	500	14/14	0.97	0.10	0.91	14,16,18,19	0
2	ZDP	E	500	14/14	0.97	0.11	0.48	18,19,21,21	0
2	ZDP	B	500	14/14	0.98	0.12	0.21	14,14,17,17	0
2	ZDP	F	500	14/14	0.97	0.09	-0.11	20,21,24,24	0
2	ZDP	D	500	14/14	0.98	0.09	-0.39	16,18,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.