



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:25 PM UTC

PDB ID : 2A0F / pdb_00002a0f
Title : Structure of D236A mutant E. coli Aspartate Transcarbamoylase in presence of Phosphonoacetamide at 2.90 Å resolution
Authors : Stieglitz, K.A.; Dusinger, K.J.; Cardia, J.P.; Tsuruta, H.; Kantrowitz, E.R.
Deposited on : 2005-06-16
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

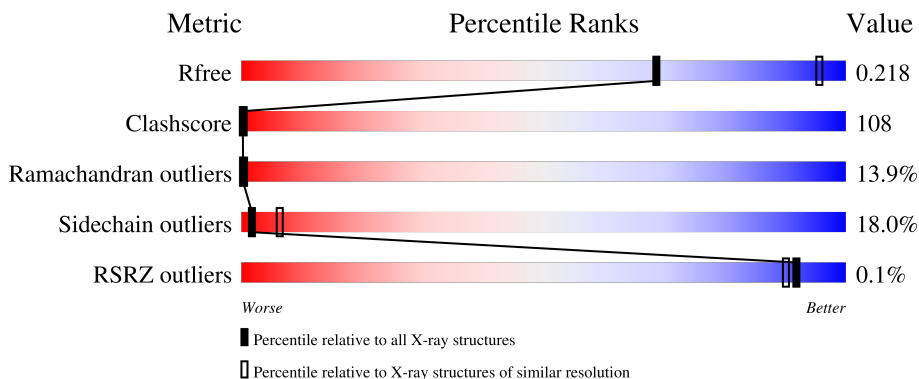
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	310	 11% 59% 26% •
1	C	310	 12% 59% 26% •
2	B	153	 17% 57% 18% • 5%
2	D	153	 12% 59% 22% • 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7489 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	Total	C	N	O	S	0	0	0
			2412	1526	423	454	9			
1	C	310	Total	C	N	O	S	0	0	0
			2412	1526	423	454	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	ASP	engineered mutation	UNP P0A786
C	236	ALA	ASP	engineered mutation	UNP P0A786

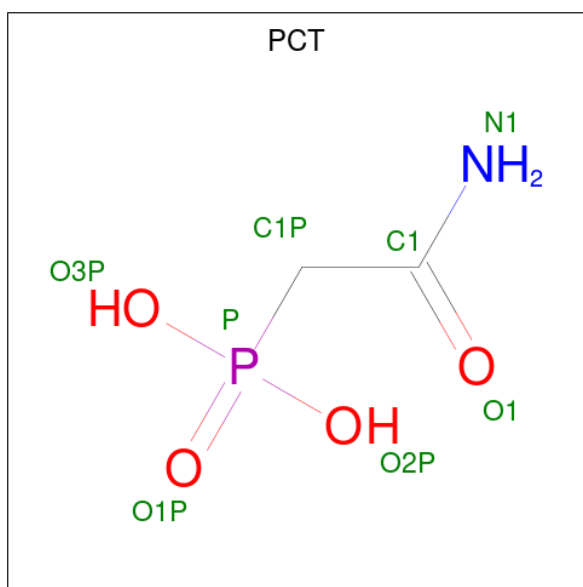
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P0A7F3
D	1	MET	-	initiating methionine	UNP P0A7F3

- Molecule 3 is PHOSPHONOACETAMIDE (CCD ID: PCT) (formula: C₂H₆NO₄P).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	B	1	1	1	0	0
4	D	1	1	1	0	0


- Molecule 5 is water.

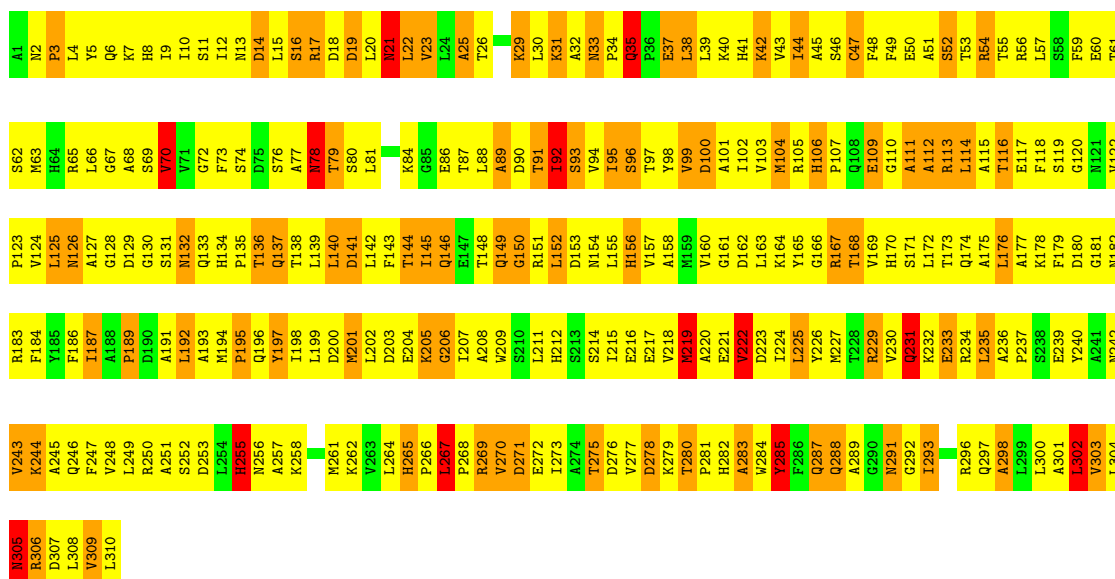
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	130	130	130	0	0
5	B	82	82	82	0	0
5	C	110	110	110	0	0
5	D	57	57	57	0	0

3 Residue-property plots

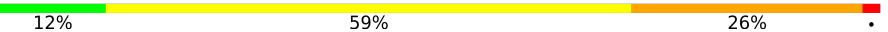
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

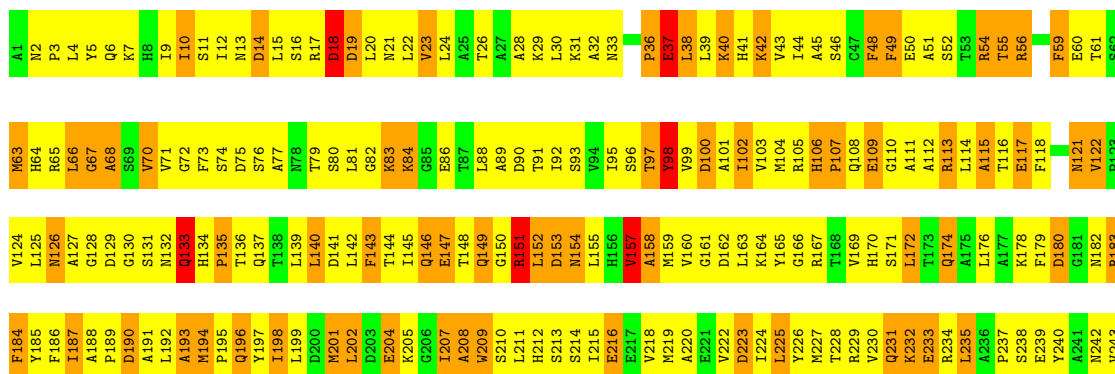
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain A: 



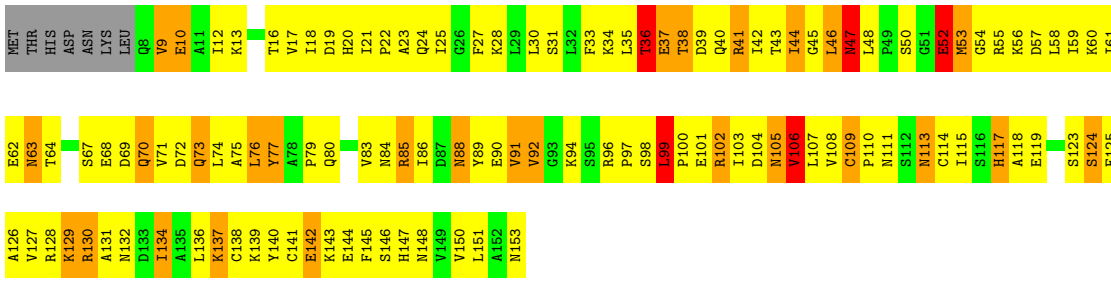
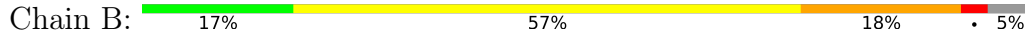
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C: 

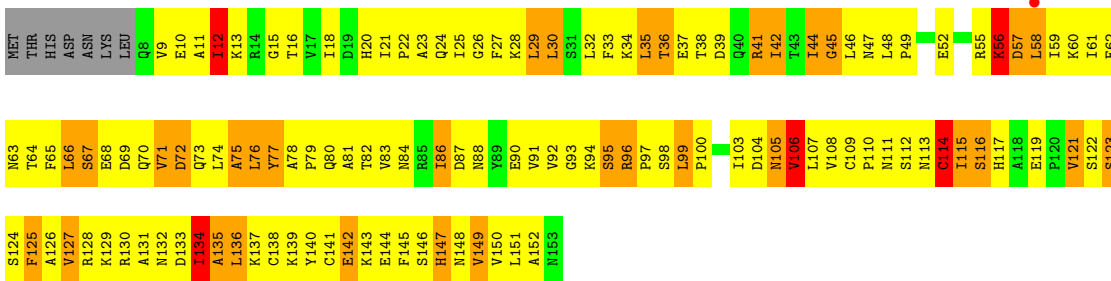
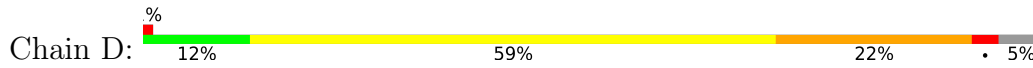




• Molecule 2: Aspartate carbamoyltransferase regulatory chain



• Molecule 2: Aspartate carbamoyltransferase regulatory chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.45Å 120.45Å 155.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.90) 83.0 (30.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.279 0.207 , 0.218	Depositor DCC
R_{free} test set	2697 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtrriage
Anisotropy	0.131	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 669.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.427 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ZN, PCT

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	0/2458	1.29	42/3335 (1.3%)
1	C	0.62	0/2458	1.07	19/3335 (0.6%)
2	B	0.68	0/1155	1.07	7/1561 (0.4%)
2	D	0.56	0/1155	1.04	8/1561 (0.5%)
All	All	0.67	0/7226	1.15	76/9792 (0.8%)

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	A	0	1

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	VAL	CA-C-N	9.90	130.00	119.90
1	C	122	VAL	C-N-CA	9.90	130.00	119.90
1	C	198	ILE	N-CA-C	-9.78	98.58	113.16
1	A	33	ASN	CA-C-N	9.78	132.07	119.84
1	A	33	ASN	C-N-CA	9.78	132.07	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	TYR	Sidechain

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	2412	0	2423	479	0
1	C	2412	0	2423	602	0
2	B	1138	0	1152	216	0
2	D	1138	0	1154	306	0
3	A	8	0	4	3	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	130	0	0	22	0
5	B	82	0	0	18	0
5	C	110	0	0	33	0
5	D	57	0	0	3	0
All	All	7489	0	7156	1544	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 108.

The worst 5 of 1544 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)
2:D:111:ASN:HD22	2:D:114:CYS:HB2	1.07	1.16
1:A:158:ALA:HB2	1:A:222:VAL:HG11	1.26	1.11
1:C:159:MET:HE3	1:C:172:LEU:HD23	1.31	1.08
2:D:82:THR:HA	2:D:96:ARG:HH12	1.11	1.08
2:B:44:ILE:HG23	2:D:44:ILE:HB	1.37	1.06

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	308/310 (99%)	200 (65%)	73 (24%)	35 (11%)	0	1
1	C	308/310 (99%)	187 (61%)	70 (23%)	51 (17%)	0	0
2	B	144/153 (94%)	82 (57%)	44 (31%)	18 (12%)	0	0
2	D	144/153 (94%)	88 (61%)	34 (24%)	22 (15%)	0	0
All	All	904/926 (98%)	557 (62%)	221 (24%)	126 (14%)	0	0

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	21	ASN
1	A	192	LEU
1	A	231	GLN
1	A	244	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	260/260 (100%)	206 (79%)	54 (21%)	1	4
1	C	260/260 (100%)	216 (83%)	44 (17%)	2	7
2	B	129/137 (94%)	107 (83%)	22 (17%)	2	7
2	D	129/137 (94%)	109 (84%)	20 (16%)	2	9
All	All	778/794 (98%)	638 (82%)	140 (18%)	2	6

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	275	THR
1	C	310	LEU
2	D	76	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	287	GLN
1	A	285	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	63	ASN
2	D	111	ASN
2	B	132	ASN
2	D	148	ASN
2	D	24	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	PCT	A	1311	-	7,7,7	2.90	4 (57%)	9,10,10	0.93	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	PCT	A	1311	-	-	1/4/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1311	PCT	P-O1P	5.60	1.61	1.50
3	A	1311	PCT	P-O2P	-3.57	1.47	1.55
3	A	1311	PCT	P-O3P	3.02	1.61	1.55
3	A	1311	PCT	P-C1P	2.02	1.82	1.79

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1311	PCT	O1-C1-C1P-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1311	PCT	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	310/310 (100%)	-1.47	0 100 100	13, 49, 72, 89	0
1	C	310/310 (100%)	-1.28	0 100 100	60, 90, 112, 137	0
2	B	146/153 (95%)	-1.33	0 100 100	41, 78, 98, 102	0
2	D	146/153 (95%)	-1.26	1 (0%) 84 79	84, 104, 121, 127	0
All	All	912/926 (98%)	-1.35	1 (0%) 92 90	13, 82, 115, 137	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	58	LEU	2.4

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
3	PCT	A	1311	8/8	0.99	0.04	32,36,38,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	B	154	1/1	1.00	0.01	45,45,45,45	0
4	ZN	D	154	1/1	1.00	0.01	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.