



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2021 – 01:51 AM EDT

PDB ID : 1TU0
Title : Aspartate Transcarbamoylase Catalytic Chain Mutant E50A Complex with Phosphonoacetamide
Authors : Stieglitz, K.; Stec, B.; Baker, D.P.; Kantrowitz, E.R.
Deposited on : 2004-06-23
Resolution : 2.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

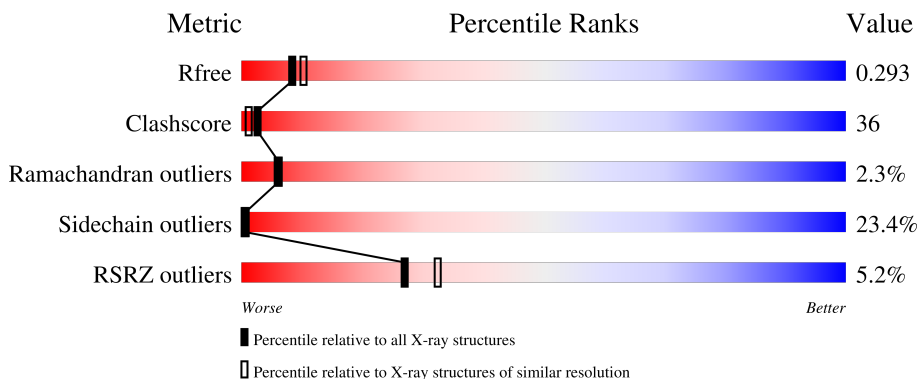
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	
1	C	310	
2	B	153	
2	D	153	

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
3	PCT	C	1312	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7596 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	2411	1525	423	454	9	0	0	0
1	C	310	2411	1525	423	454	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	ALA	GLU	engineered mutation	UNP P0A786
C	50	ALA	GLU	engineered mutation	UNP P0A786

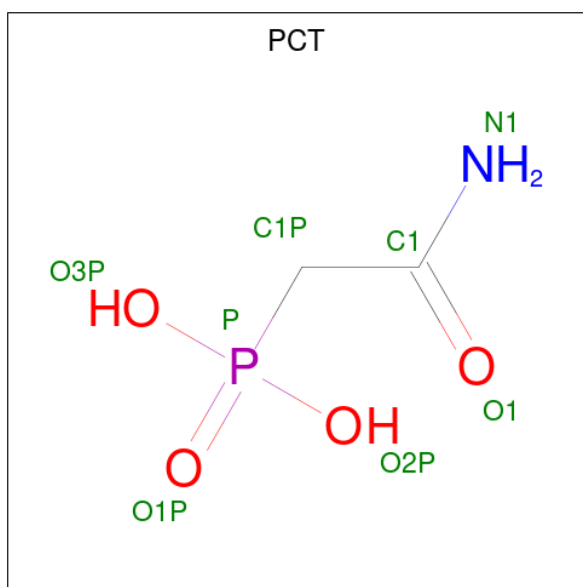
- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	153	1201	752	213	230	6	0	0	0
2	D	153	1201	752	213	230	6	0	0	0

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 (three-letter code: PCT) (formula: C₂H₆NO₄P).



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

- Molecule 4 is ZINC ION (three-letter code: 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

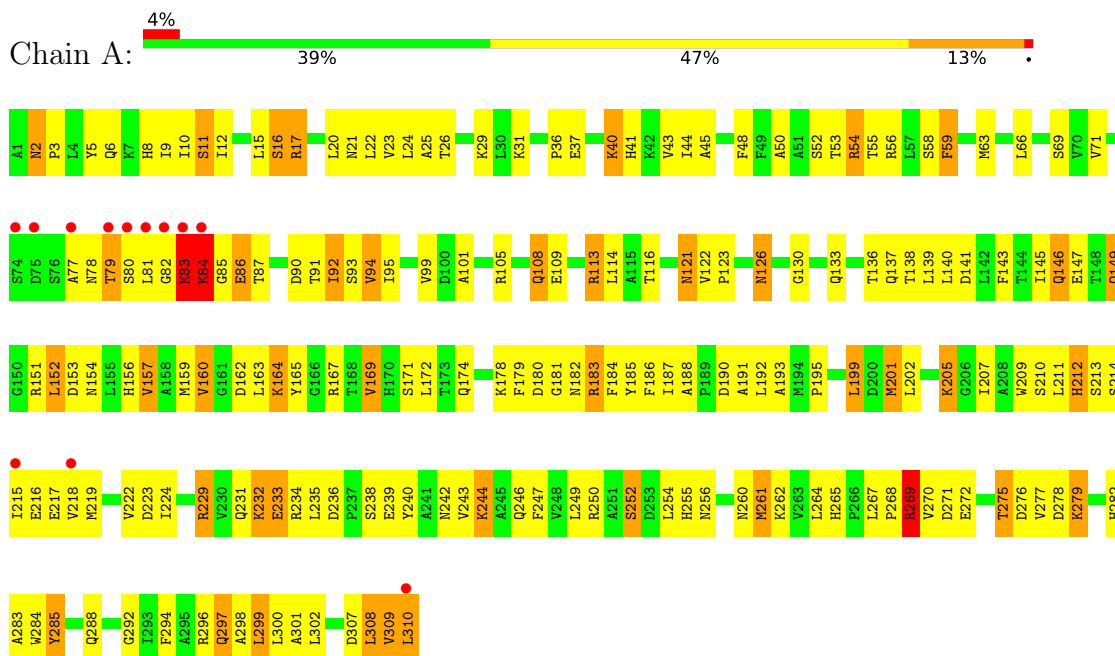
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	119	119	119	0	0
5	B	53	53	53	0	0
5	C	131	131	131	0	0
5	D	51	51	51	0	0

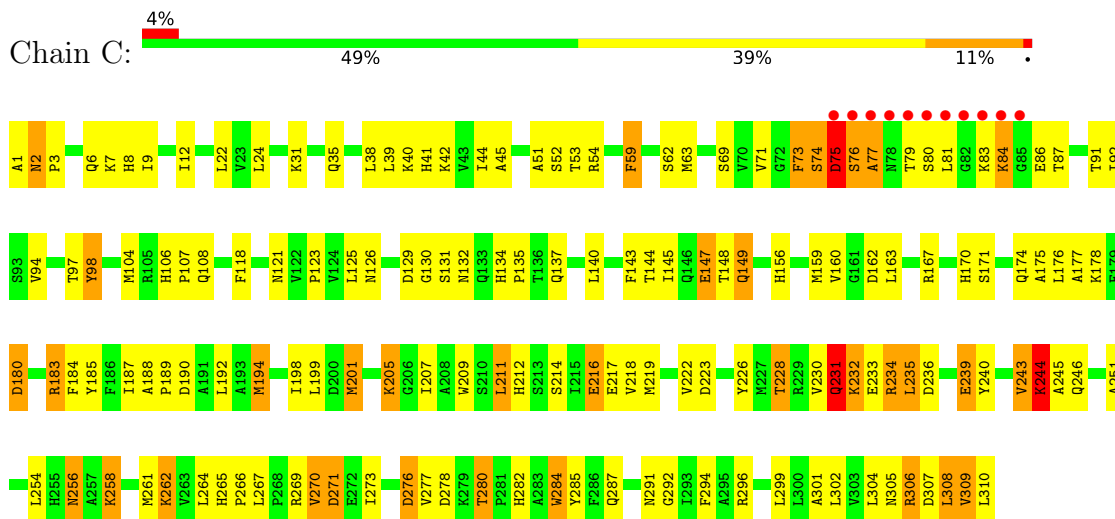
3 Residue-property plots

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.

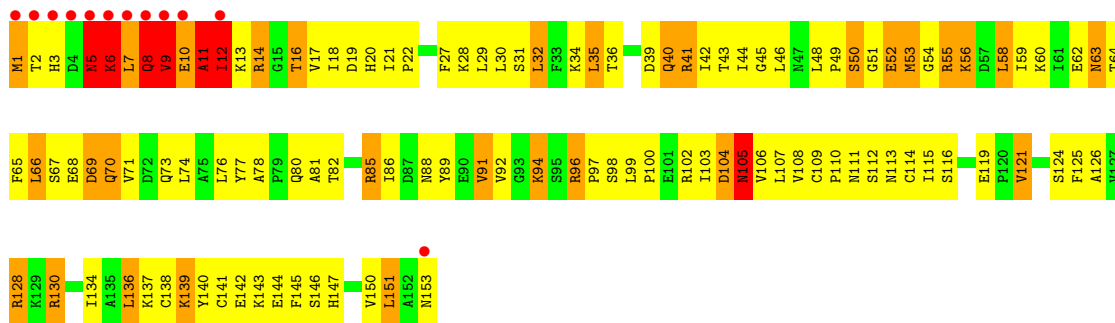
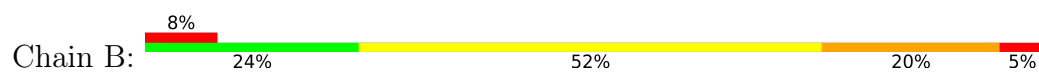
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



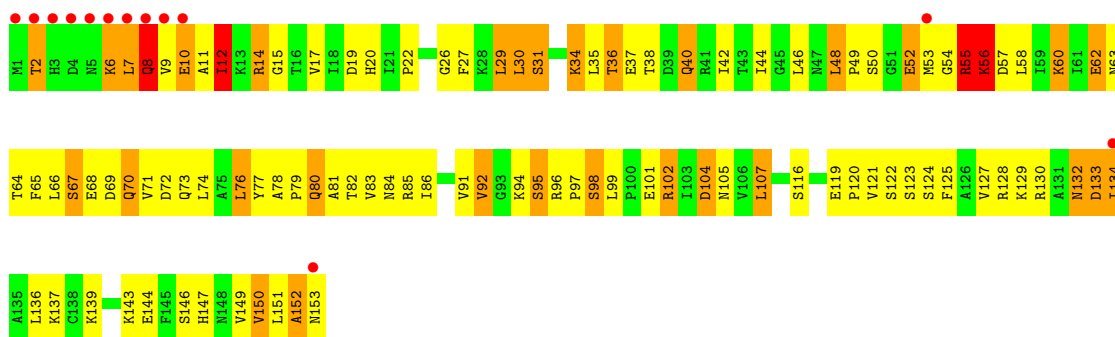
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



- 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	122.20Å 122.20Å 142.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.55 61.10 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.00-2.55) 97.8 (61.10-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.55Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.211 , 0.279 0.213 , 0.293	Depositor DCC
R_{free} test set	1994 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 392.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7596	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: PCT, ZN

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	0.49	2/2457 (0.1%)	1.03	11/3334 (0.3%)
1	C	0.44	3/2457 (0.1%)	1.06	12/3334 (0.4%)
2	B	1.34	8/1219 (0.7%)	1.21	12/1647 (0.7%)
2	D	0.76	6/1219 (0.5%)	1.11	15/1647 (0.9%)
All	All	0.73	19/7352 (0.3%)	1.08	50/9962 (0.5%)

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	3
1	C	0	1
2	B	0	3
2	D	0	2
All	All	0	9

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	ASN	N-CA	20.81	1.88	1.46
2	B	8	GLN	C-N	-17.65	0.93	1.34
2	B	105	ASN	C-N	17.59	1.74	1.34
2	B	9	VAL	C-N	17.00	1.73	1.34
2	D	152	ALA	C-N	15.67	1.70	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	309	VAL	O-C-N	-18.13	93.69	122.70
2	B	8	GLN	O-C-N	17.52	150.73	122.70
2	B	8	GLN	CA-C-N	-16.20	81.57	117.20
2	D	8	GLN	O-C-N	13.04	143.56	122.70
1	C	309	VAL	CA-C-N	11.46	142.41	117.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	LYS	Mainchain
1	A	84	LYS	Mainchain,Peptide
2	B	11	ALA	Mainchain
2	B	128	ARG	Mainchain
2	B	8	GLN	Mainchain

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	2411	0	2420	177	0
1	C	2411	0	2418	116	0
2	B	1201	0	1215	133	5
2	D	1201	0	1215	111	0
3	A	8	0	4	1	0
3	C	8	0	4	6	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	119	0	0	9	0
5	B	53	0	0	11	0
5	C	131	0	0	6	5
5	D	51	0	0	9	0
All	All	7596	0	7276	525	5

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 36.

The worst 5 of 525 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:A:309:VAL:C	1:A:310:LEU:N	1.69	1.45
2:D:152:ALA:C	2:D:153:ASN:N	1.70	1.42
2:B:9:VAL:C	2:B:10:GLU:N	1.73	1.42
2:B:105:ASN:C	2:B:106:VAL:N	1.74	1.39
2:B:105:ASN:N	2:B:105:ASN:CA	1.88	1.36

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:SER:OG	5:C:1441:HOH:O[2_655]	1.16	1.04
2:B:144:GLU:O	5:C:1425:HOH:O[2_655]	1.47	0.73
2:B:112:SER:N	5:C:1441:HOH:O[2_655]	1.92	0.28
2:B:112:SER:CB	5:C:1441:HOH:O[2_655]	1.95	0.25
2:B:112:SER:CA	5:C:1441:HOH:O[2_655]	2.18	0.02

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%)	274 (89%)	31 (10%)	3 (1%)	15	22
1	C	308/310 (99%)	276 (90%)	24 (8%)	8 (3%)	5	5
2	B	151/153 (99%)	130 (86%)	15 (10%)	6 (4%)	3	1
2	D	151/153 (99%)	128 (85%)	19 (13%)	4 (3%)	5	5
All	All	918/926 (99%)	808 (88%)	89 (10%)	21 (2%)	6	6

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	THR
2	B	6	LYS

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Mol	Chain	Res	Type
2	B	13	LYS
1	C	75	ASP
1	C	270	VAL

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%)	204 (78%)	56 (22%)	1	1
1	C	260/260 (100%)	206 (79%)	54 (21%)	1	1
2	B	137/137 (100%)	97 (71%)	40 (29%)	0	0
2	D	137/137 (100%)	101 (74%)	36 (26%)	0	0
All	All	794/794 (100%)	608 (77%)	186 (23%)	1	0

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	134	HIS
1	C	280	THR
1	C	171	SER
1	C	231	GLN
2	D	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	111	ASN
2	D	80	GLN
1	C	21	ASN
2	D	20	HIS
2	B	147	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	3.01	4 (57%)	9,10,10	1.59	1 (11%)
3	PCT	C	1312	-	7,7,7	3.03	4 (57%)	9,10,10	1.59	2 (22%)

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	-	-	0/4/5/5	-
3	PCT	C	1312	-	-	2/4/5/5	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1312	PCT	P-O1P	5.15	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1311	PCT	P-O1P	5.10	1.60	1.50
3	C	1312	PCT	P-C1P	4.31	1.86	1.79
3	A	1311	PCT	P-C1P	4.28	1.86	1.79
3	C	1312	PCT	P-O3P	3.41	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1312	PCT	O1-C1-C1P	3.13	122.92	119.72
3	A	1311	PCT	O1-C1-C1P	2.21	121.98	119.72
3	C	1312	PCT	O1P-P-C1P	-2.07	106.22	110.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1312	PCT	O1-C1-C1P-P
3	C	1312	PCT	C1-C1P-P-O3P

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1311	PCT	1	0
3	C	1312	PCT	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	5
2	D	2
1	C	2
1	A	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	105:ASN	C	106:VAL	N	1.74
1	B	9:VAL	C	10:GLU	N	1.73
1	D	152:ALA	C	153:ASN	N	1.70
1	A	309:VAL	C	310:LEU	N	1.69
1	B	5:ASN	C	6:LYS	N	1.67

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%)	-0.27	12 (3%) 39 45	3, 27, 104, 158	0
1	C	310/310 (100%)	-0.43	11 (3%) 44 51	2, 20, 95, 158	0
2	B	153/153 (100%)	0.22	12 (7%) 13 16	11, 49, 158, 158	1 (0%)
2	D	153/153 (100%)	0.42	13 (8%) 10 12	10, 55, 158, 158	3 (1%)
All	All	926/926 (100%)	-0.12	48 (5%) 27 32	2, 35, 141, 158	4 (0%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	THR	8.6
2	B	1	MET	7.6
2	B	9	VAL	7.4
2	D	5	ASN	7.1
1	A	79	THR	6.9

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 monosaccharides 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(\AA^2)	Q<0.9
3	PCT	C	1312	8/8	0.89	0.20	54,64,75,87	0
3	PCT	A	1311	8/8	0.90	0.25	24,54,73,78	0
4	ZN	B	154	1/1	0.99	0.04	19,19,19,19	0
4	ZN	D	155	1/1	0.99	0.05	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.