



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2017 – 07:51 AM EDT

PDB ID : 3TCM
Title : Crystal Structure of Alanine Aminotransferase from *Hordeum vulgare*
Authors : Rydel, T.J.; Sturman, E.J.; Halls, C.; Chen, S.; Zeng, J.; Evdokimov, A.; Duff, S.M.G.
Deposited on : unknown
Resolution : 2.71 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

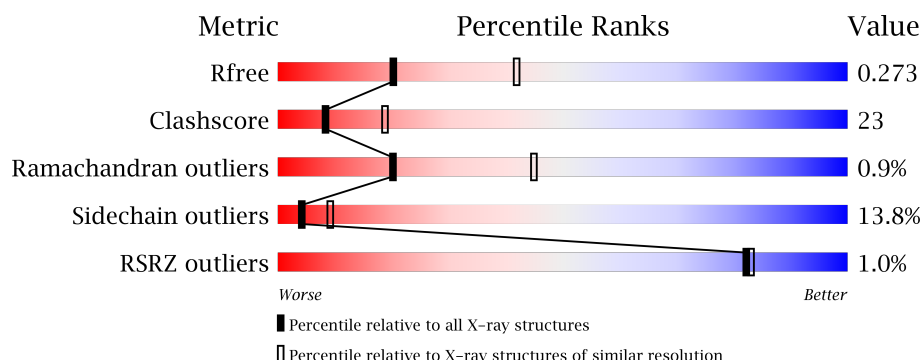
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	100719	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (2.74-2.70)

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	500	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 59%, yellow 29%, orange 7%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 100% 59% 29% 7% • • </div> </div>
1	B	500	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 26%, orange 8%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 100% 61% 26% 8% • • </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7514 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 Alanine aminotransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	1	0
			3706	2360	633	697	16			
1	B	479	Total	C	N	O	S	0	0	0
			3703	2358	633	697	15			

There are 38 discrepancies between the modelled and reference sequences:

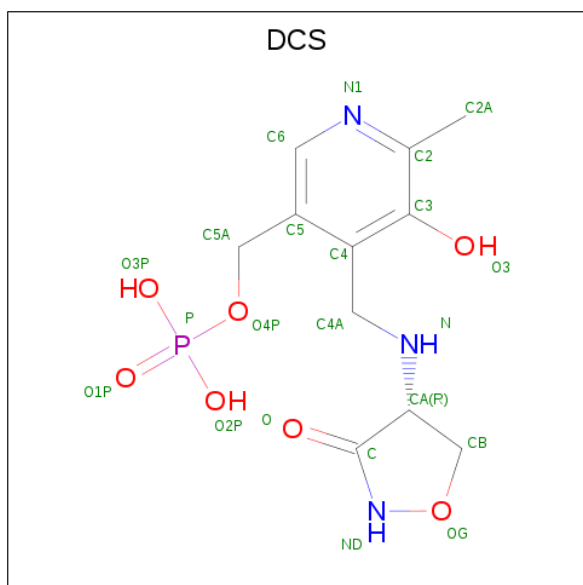
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	INITIATING METHIONINE	UNP P52894
A	-16	HIS	-	EXPRESSION TAG	UNP P52894
A	-15	HIS	-	EXPRESSION TAG	UNP P52894
A	-14	HIS	-	EXPRESSION TAG	UNP P52894
A	-13	HIS	-	EXPRESSION TAG	UNP P52894
A	-12	HIS	-	EXPRESSION TAG	UNP P52894
A	-11	HIS	-	EXPRESSION TAG	UNP P52894
A	-10	HIS	-	EXPRESSION TAG	UNP P52894
A	-9	HIS	-	EXPRESSION TAG	UNP P52894
A	-8	HIS	-	EXPRESSION TAG	UNP P52894
A	-7	HIS	-	EXPRESSION TAG	UNP P52894
A	-6	GLY	-	EXPRESSION TAG	UNP P52894
A	-5	THR	-	EXPRESSION TAG	UNP P52894
A	-4	ASP	-	EXPRESSION TAG	UNP P52894
A	-3	ASP	-	EXPRESSION TAG	UNP P52894
A	-2	ASP	-	EXPRESSION TAG	UNP P52894
A	-1	ASP	-	EXPRESSION TAG	UNP P52894
A	0	LYS	-	EXPRESSION TAG	UNP P52894
A	119	HIS	LYS	ENGINEERED MUTATION	UNP P52894
B	-17	MET	-	INITIATING METHIONINE	UNP P52894
B	-16	HIS	-	EXPRESSION TAG	UNP P52894
B	-15	HIS	-	EXPRESSION TAG	UNP P52894
B	-14	HIS	-	EXPRESSION TAG	UNP P52894
B	-13	HIS	-	EXPRESSION TAG	UNP P52894
B	-12	HIS	-	EXPRESSION TAG	UNP P52894

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	EXPRESSION TAG	UNP P52894
B	-10	HIS	-	EXPRESSION TAG	UNP P52894
B	-9	HIS	-	EXPRESSION TAG	UNP P52894
B	-8	HIS	-	EXPRESSION TAG	UNP P52894
B	-7	HIS	-	EXPRESSION TAG	UNP P52894
B	-6	GLY	-	EXPRESSION TAG	UNP P52894
B	-5	THR	-	EXPRESSION TAG	UNP P52894
B	-4	ASP	-	EXPRESSION TAG	UNP P52894
B	-3	ASP	-	EXPRESSION TAG	UNP P52894
B	-2	ASP	-	EXPRESSION TAG	UNP P52894
B	-1	ASP	-	EXPRESSION TAG	UNP P52894
B	0	LYS	-	EXPRESSION TAG	UNP P52894
B	119	HIS	LYS	ENGINEERED MUTATION	UNP P52894

- Molecule 2 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (three-letter code: DCS) (formula: $C_{11}H_{16}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

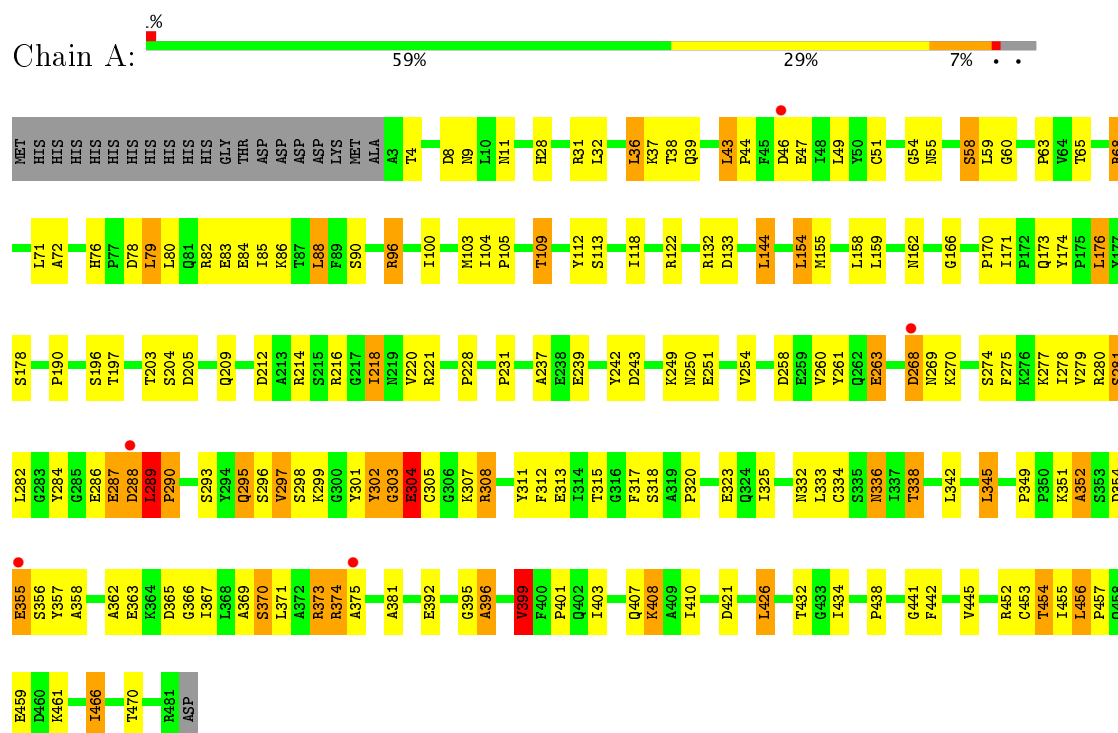
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	32	Total 32	O 32	0	0

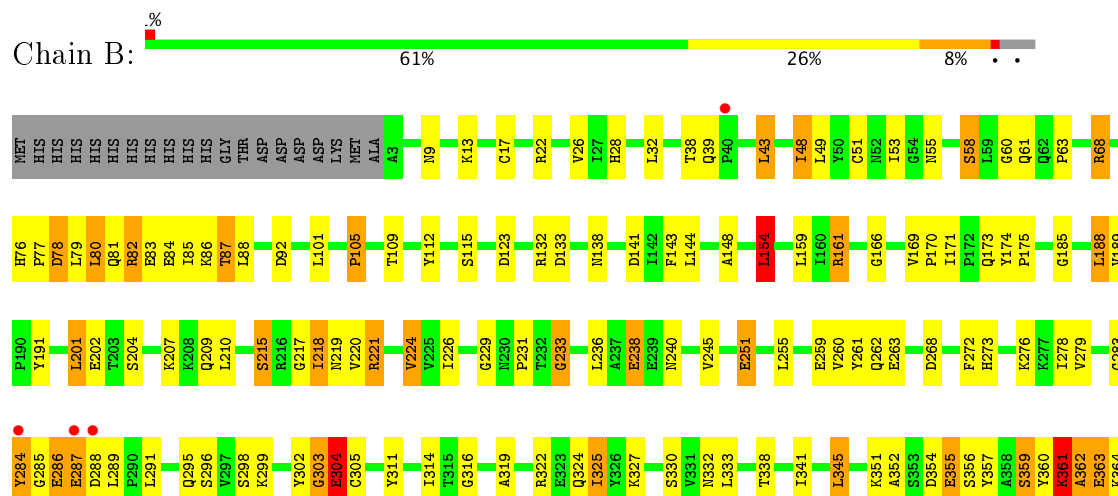
3 Residue-property plots

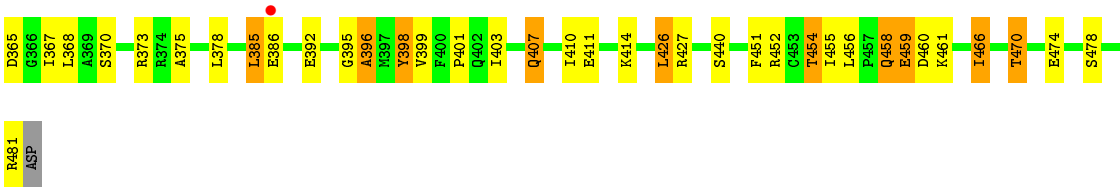
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Alanine aminotransferase 2



• Molecule 1: Alanine aminotransferase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	119.86 Å 126.97 Å 75.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.16 – 2.71 36.26 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.8 (87.16-2.71) 96.9 (36.26-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.72 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.279 0.212 , 0.273	Depositor DCC
R_{free} test set	1582 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7514	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: DCS

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	1.07	2/3788 (0.1%)	1.06	18/5135 (0.4%)
1	B	1.13	4/3782 (0.1%)	1.10	21/5127 (0.4%)
All	All	1.10	6/7570 (0.1%)	1.08	39/10262 (0.4%)

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	2
1	B	0	1
All	All	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	GLU	CG-CD	6.00	1.60	1.51
1	B	398	TYR	CE1-CZ	-5.84	1.30	1.38
1	A	297	VAL	CB-CG1	-5.51	1.41	1.52
1	B	407	GLN	CD-OE1	5.38	1.35	1.24
1	B	411	GLU	CG-CD	5.30	1.59	1.51

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	LYS	N-CA-CB	-17.20	79.64	110.60
1	A	303	GLY	N-CA-C	9.19	136.07	113.10
1	A	289	LEU	N-CA-C	-9.18	86.22	111.00
1	A	303	GLY	C-N-CA	9.09	144.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	GLY	N-CA-C	8.71	134.88	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	SER	Peptide
1	A	441	GLY	Peptide
1	B	161	ARG	Peptide

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	3706	0	3696	177	0
1	B	3703	0	3694	182	0
2	A	22	0	13	6	0
2	B	22	0	14	3	0
3	A	29	0	0	3	0
3	B	32	0	0	2	0
All	All	7514	0	7417	345	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 23.

The worst 5 of 345 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:82:ARG:CB	1:B:82:ARG:HH11	1.43	1.29
1:B:284:TYR:CD1	1:B:288:ASP:OD1	1.90	1.24
1:B:284:TYR:CG	1:B:288:ASP:CG	2.12	1.23
1:B:303:GLY:HA2	1:B:304:GLU:CB	1.56	1.21
1:B:92:ASP:OD1	1:B:356:SER:HB2	1.42	1.18

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	478/500 (96%)	450 (94%)	24 (5%)	4 (1%)	22	48
1	B	477/500 (95%)	446 (94%)	26 (6%)	5 (1%)	18	41
All	All	955/1000 (96%)	896 (94%)	50 (5%)	9 (1%)	20	45

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	GLU
1	B	283	GLY
1	B	304	GLU
1	A	352	ALA
1	A	396	ALA

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	396/414 (96%)	339 (86%)	57 (14%)	4	8
1	B	395/414 (95%)	343 (87%)	52 (13%)	5	10
All	All	791/828 (96%)	682 (86%)	109 (14%)	4	9

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	LYS

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Mol	Chain	Res	Type
1	B	68	ARG
1	B	414	LYS
1	A	426	LEU
1	A	461	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

2 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	DCS	A	501	-	23,23,23	3.29	8 (34%)	25,33,33	1.86	5 (20%)
2	DCS	B	502	-	23,23,23	3.32	6 (26%)	25,33,33	2.36	11 (44%)

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	DCS	A	501	-	-	0/10/21/21	0/2/2/2
2	DCS	B	502	-	-	0/10/21/21	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	DCS	CA-C	-8.28	1.46	1.52
2	A	501	DCS	OG-ND	-4.77	1.35	1.45
2	B	502	DCS	OG-ND	-4.46	1.36	1.45
2	B	502	DCS	C-ND	-2.46	1.31	1.34
2	A	501	DCS	C-ND	-2.45	1.31	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	DCS	O-C-CA	-4.39	123.09	126.23
2	B	502	DCS	O3P-P-O4P	-2.95	98.90	106.73
2	B	502	DCS	C4-C3-C2	-2.71	115.35	120.04
2	B	502	DCS	O-C-CA	-2.49	124.45	126.23
2	B	502	DCS	C3-C4-C5	-2.18	116.56	118.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	DCS	6	0
2	B	502	DCS	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	479/500 (95%)	-0.15	5 (1%) 82 83	24, 40, 61, 76	0
1	B	479/500 (95%)	-0.02	5 (1%) 82 83	24, 39, 61, 76	0
All	All	958/1000 (95%)	-0.09	10 (1%) 82 83	24, 40, 61, 76	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ASP	6.9
1	A	355	GLU	3.9
1	A	288	ASP	3.7
1	B	284	TYR	3.5
1	A	375	ALA	2.7

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(\AA^2)	Q<0.9
2	DCS	A	501	22/22	0.98	0.19	0.42	27,32,38,39	0
2	DCS	B	502	22/22	0.98	0.24	0.11	26,33,42,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.