



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2019 – 06:15 AM EST

PDB ID : 6CSF
Title : Crystal structure of sodium/alanine symporter AgcS with D-alanine bound
Authors : Ma, J.; Reyes, F.E.; Gonen, T.
Deposited on : 2018-03-20
Resolution : 3.30 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

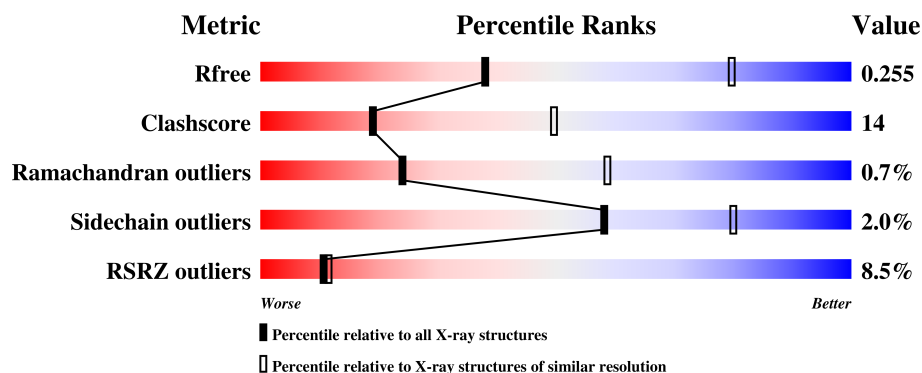
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)

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	214	<div> <div>14%</div> <div>78%21%</div> </div>
1	H	214	<div> <div>6%</div> <div>78%21%</div> </div>
2	B	213	<div> <div>3%</div> <div>78%21%</div> </div>
2	L	213	<div> <div>7%</div> <div>82%18%</div> </div>
3	C	453	<div> <div>10%</div> <div>61%32%6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	453	 A horizontal bar chart showing the quality of chain 3. The bar is divided into four segments: a small red segment at the beginning labeled '8%', followed by a large green segment labeled '65%', then a yellow segment labeled '29%', and a very small grey segment at the end labeled '5%'.

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
5	DAL	M	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12670 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 Monoclonal antibody FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1556	973	259	315	9			
1	H	214	Total	C	N	O	S	0	0	0
			1556	973	259	315	9			

- Molecule 2 is a protein called Monoclonal antibody FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1606	998	273	328	7			
2	L	213	Total	C	N	O	S	0	0	0
			1606	998	273	328	7			

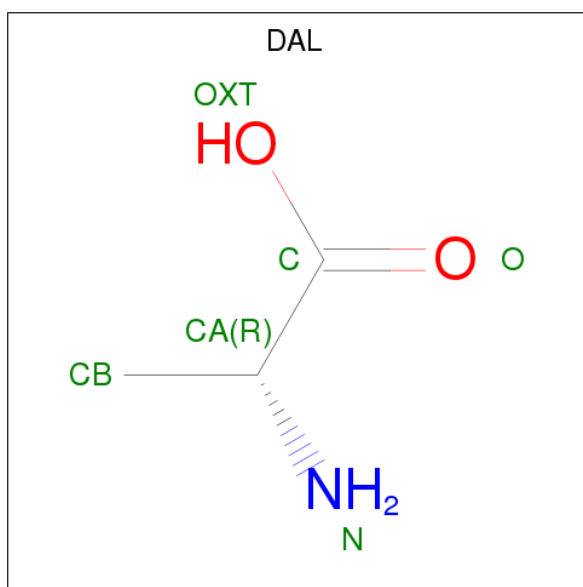
- Molecule 3 is a protein called Sodium/alanine symporter AgcS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	431	Total	C	N	O	S	0	0	0
			3183	2113	498	555	17			
3	C	428	Total	C	N	O	S	0	0	0
			3156	2094	495	550	17			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Na	0	0
			1	1		

- Molecule 5 is D-ALANINE (three-letter code: DAL) (formula: C₃H₇NO₂).

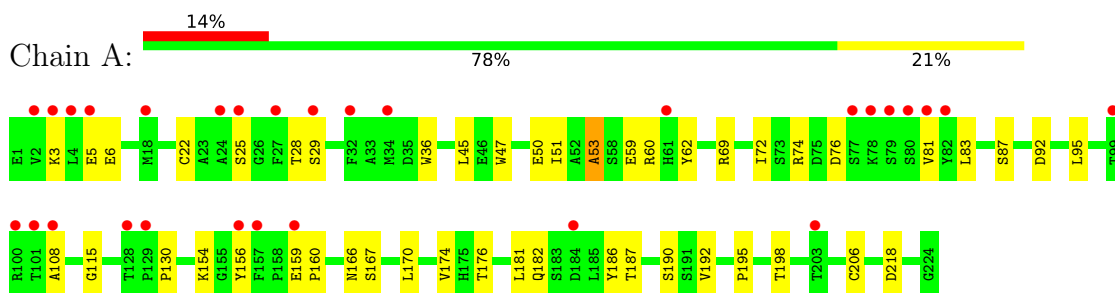


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	6	3	1	2	0	0

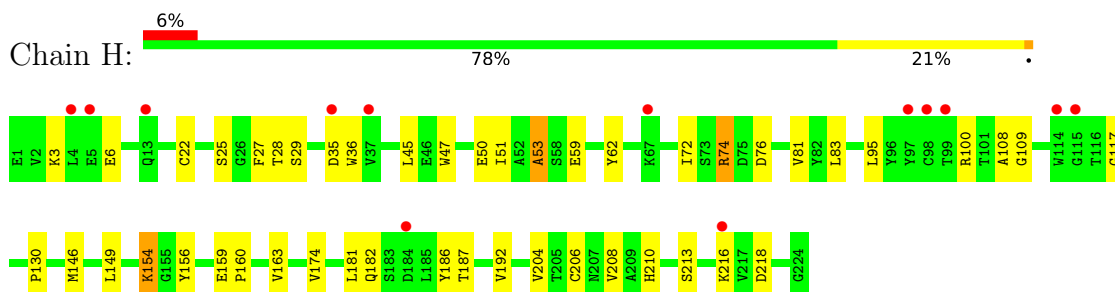
3 Residue-property plots [i](#)

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.

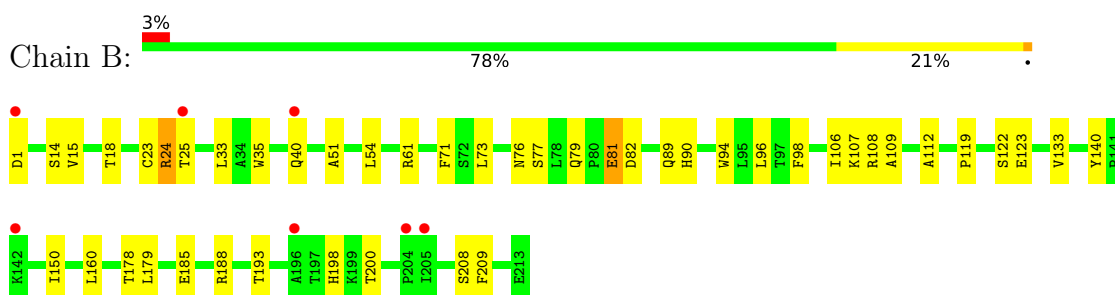
- Molecule 1: Monoclonal antibody FAB heavy chain



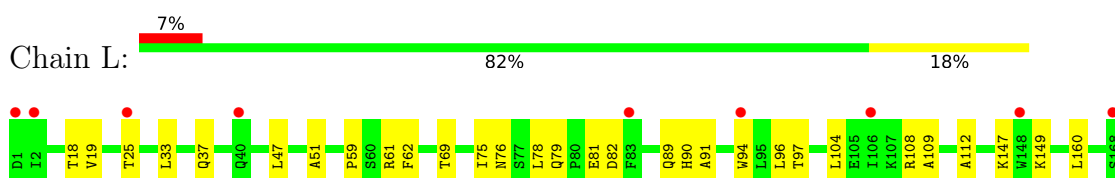
- Molecule 1: Monoclonal antibody FAB heavy chain

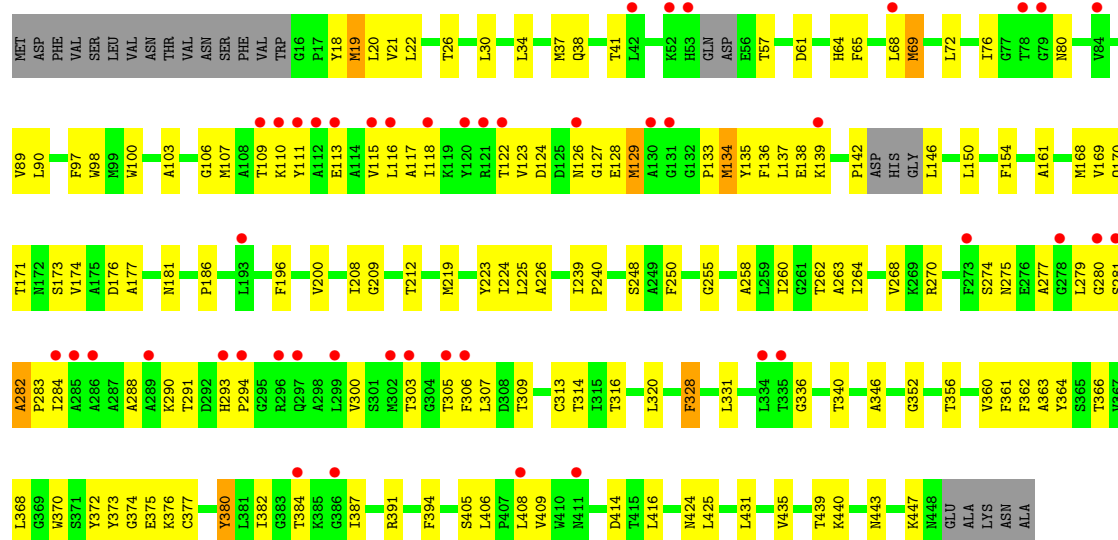


- Molecule 2: Monoclonal antibody FAB light chain



- Molecule 2: Monoclonal antibody FAB light chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	183.05Å 183.05Å 349.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	158.53 – 3.30 158.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (158.53-3.30) 99.9 (158.53-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.240 , 0.253 0.241 , 0.255	Depositor DCC
R_{free} test set	4920 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	112.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	12670	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

5.1 Standard geometry

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

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	0.33	0/1593	0.56	0/2177
1	H	0.32	0/1593	0.55	0/2177
2	B	0.29	0/1639	0.55	0/2225
2	L	0.30	0/1639	0.55	0/2225
3	C	0.35	0/3229	0.48	0/4390
3	M	0.28	0/3257	0.47	0/4428
All	All	0.31	0/12950	0.52	0/17622

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1556	0	1510	33	0
1	H	1556	0	1510	31	0
2	B	1606	0	1554	40	0
2	L	1606	0	1554	33	0
3	C	3156	0	3246	127	0
3	M	3183	0	3272	107	0
4	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	6	0	6	8	0
All	All	12670	0	12652	355	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 14.

The worst 5 of 355 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)
3:C:284:ILE:HG21	3:C:373:TYR:HA	1.39	1.04
3:C:282:ALA:H	3:C:283:PRO:HD2	1.26	1.00
3:C:281:SER:O	3:C:373:TYR:CE2	2.20	0.95
3:C:282:ALA:H	3:C:283:PRO:CD	1.82	0.92
3:M:77:GLY:HA3	5:M:502:DAL:O	1.73	0.88

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	212/214 (99%)	202 (95%)	8 (4%)	2 (1%)	19	53
1	H	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	19	53
2	B	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
2	L	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
3	C	422/453 (93%)	386 (92%)	29 (7%)	7 (2%)	10	40
3	M	425/453 (94%)	402 (95%)	22 (5%)	1 (0%)	49	80
All	All	1693/1760 (96%)	1598 (94%)	83 (5%)	12 (1%)	24	59

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	53	ALA
3	C	186	PRO
1	A	53	ALA
1	A	108	ALA
1	H	108	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	172/172 (100%)	170 (99%)	2 (1%)	74	86
1	H	172/172 (100%)	168 (98%)	4 (2%)	53	78
2	B	179/179 (100%)	175 (98%)	4 (2%)	55	79
2	L	179/179 (100%)	179 (100%)	0	100	100
3	C	315/337 (94%)	306 (97%)	9 (3%)	45	74
3	M	317/337 (94%)	309 (98%)	8 (2%)	50	76
All	All	1334/1376 (97%)	1307 (98%)	27 (2%)	58	80

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	394	PHE
1	H	76	ASP
3	C	380	TYR
3	M	446	ARG
2	B	54	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	424	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 [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
5	DAL	M	502	-	2,5,5	0.54	0	2,6,6	0.73	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
5	DAL	M	502	-	-	0/0/4/4	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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	502	DAL	8	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	214/214 (100%)	0.96	29 (13%) 3 3	68, 91, 123, 177	0
1	H	214/214 (100%)	0.68	13 (6%) 21 21	68, 93, 128, 155	0
2	B	213/213 (100%)	0.57	7 (3%) 46 45	71, 96, 128, 165	0
2	L	213/213 (100%)	0.66	14 (6%) 18 19	70, 96, 127, 162	0
3	C	428/453 (94%)	0.71	46 (10%) 6 6	91, 142, 194, 245	0
3	M	431/453 (95%)	0.70	37 (8%) 10 11	86, 127, 173, 210	0
All	All	1713/1760 (97%)	0.71	146 (8%) 11 11	68, 113, 172, 245	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	137	LEU	7.1
3	C	130	ALA	6.3
3	M	121	ARG	5.3
3	M	444	GLU	5.3
3	C	293	HIS	5.2

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. 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
4	NA	M	501	1/1	0.84	0.12	113,113,113,113	0
5	DAL	M	502	6/6	0.91	0.28	126,128,135,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.