



Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2017 – 02:07 PM EDT

PDB ID : 5U0J
Title : C-terminal ankyrin repeats from human kidney-type glutaminase (KGA) - monoclinic crystal form
Authors : Pasquali, C.C.; Gonzalez, A.; Dias, S.M.G.; Ambrosio, A.L.B.
Deposited on : 2016-11-24
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
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-20029077

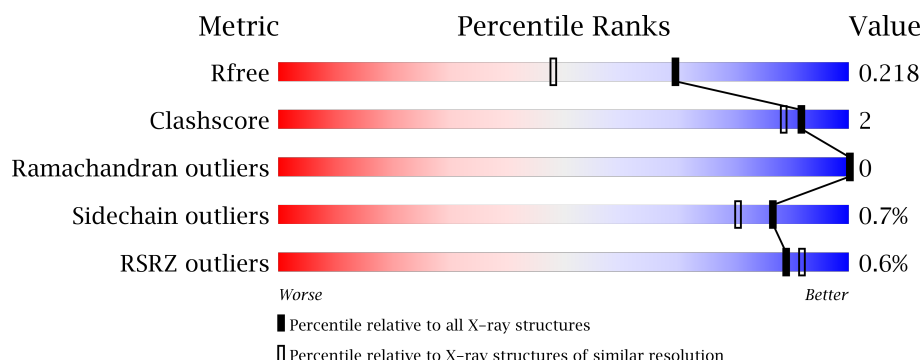
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	4385 (1.74-1.70)
Clashscore	112137	4841 (1.74-1.70)
Ramachandran outliers	110173	4771 (1.74-1.70)
Sidechain outliers	110143	4771 (1.74-1.70)
RSRZ outliers	101464	4426 (1.74-1.70)

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	140	
1	B	140	
1	C	140	
1	D	140	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3582 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	1	0
			730	465	127	134	4			
1	B	90	Total	C	N	O	S	0	2	0
			733	468	128	133	4			
1	C	90	Total	C	N	O	S	0	2	0
			738	471	128	135	4			
1	D	91	Total	C	N	O	S	0	1	0
			739	470	129	136	4			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	MET	-	initiating methionine	UNP O94925
A	531	GLY	-	expression tag	UNP O94925
A	532	SER	-	expression tag	UNP O94925
A	533	SER	-	expression tag	UNP O94925
A	534	HIS	-	expression tag	UNP O94925
A	535	HIS	-	expression tag	UNP O94925
A	536	HIS	-	expression tag	UNP O94925
A	537	HIS	-	expression tag	UNP O94925
A	538	HIS	-	expression tag	UNP O94925
A	539	HIS	-	expression tag	UNP O94925
A	540	SER	-	expression tag	UNP O94925
A	541	SER	-	expression tag	UNP O94925
A	542	GLY	-	expression tag	UNP O94925
A	543	LEU	-	expression tag	UNP O94925
A	544	VAL	-	expression tag	UNP O94925
A	545	PRO	-	expression tag	UNP O94925
A	546	ARG	-	expression tag	UNP O94925
A	547	GLY	-	expression tag	UNP O94925
A	548	SER	-	expression tag	UNP O94925
A	549	HIS	-	expression tag	UNP O94925
A	550	MET	-	expression tag	UNP O94925

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Chain	Residue	Modelled	Actual	Comment	Reference
B	530	MET	-	initiating methionine	UNP O94925
B	531	GLY	-	expression tag	UNP O94925
B	532	SER	-	expression tag	UNP O94925
B	533	SER	-	expression tag	UNP O94925
B	534	HIS	-	expression tag	UNP O94925
B	535	HIS	-	expression tag	UNP O94925
B	536	HIS	-	expression tag	UNP O94925
B	537	HIS	-	expression tag	UNP O94925
B	538	HIS	-	expression tag	UNP O94925
B	539	HIS	-	expression tag	UNP O94925
B	540	SER	-	expression tag	UNP O94925
B	541	SER	-	expression tag	UNP O94925
B	542	GLY	-	expression tag	UNP O94925
B	543	LEU	-	expression tag	UNP O94925
B	544	VAL	-	expression tag	UNP O94925
B	545	PRO	-	expression tag	UNP O94925
B	546	ARG	-	expression tag	UNP O94925
B	547	GLY	-	expression tag	UNP O94925
B	548	SER	-	expression tag	UNP O94925
B	549	HIS	-	expression tag	UNP O94925
B	550	MET	-	expression tag	UNP O94925
C	530	MET	-	initiating methionine	UNP O94925
C	531	GLY	-	expression tag	UNP O94925
C	532	SER	-	expression tag	UNP O94925
C	533	SER	-	expression tag	UNP O94925
C	534	HIS	-	expression tag	UNP O94925
C	535	HIS	-	expression tag	UNP O94925
C	536	HIS	-	expression tag	UNP O94925
C	537	HIS	-	expression tag	UNP O94925
C	538	HIS	-	expression tag	UNP O94925
C	539	HIS	-	expression tag	UNP O94925
C	540	SER	-	expression tag	UNP O94925
C	541	SER	-	expression tag	UNP O94925
C	542	GLY	-	expression tag	UNP O94925
C	543	LEU	-	expression tag	UNP O94925
C	544	VAL	-	expression tag	UNP O94925
C	545	PRO	-	expression tag	UNP O94925
C	546	ARG	-	expression tag	UNP O94925
C	547	GLY	-	expression tag	UNP O94925
C	548	SER	-	expression tag	UNP O94925
C	549	HIS	-	expression tag	UNP O94925
C	550	MET	-	expression tag	UNP O94925

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Chain	Residue	Modelled	Actual	Comment	Reference
D	530	MET	-	initiating methionine	UNP O94925
D	531	GLY	-	expression tag	UNP O94925
D	532	SER	-	expression tag	UNP O94925
D	533	SER	-	expression tag	UNP O94925
D	534	HIS	-	expression tag	UNP O94925
D	535	HIS	-	expression tag	UNP O94925
D	536	HIS	-	expression tag	UNP O94925
D	537	HIS	-	expression tag	UNP O94925
D	538	HIS	-	expression tag	UNP O94925
D	539	HIS	-	expression tag	UNP O94925
D	540	SER	-	expression tag	UNP O94925
D	541	SER	-	expression tag	UNP O94925
D	542	GLY	-	expression tag	UNP O94925
D	543	LEU	-	expression tag	UNP O94925
D	544	VAL	-	expression tag	UNP O94925
D	545	PRO	-	expression tag	UNP O94925
D	546	ARG	-	expression tag	UNP O94925
D	547	GLY	-	expression tag	UNP O94925
D	548	SER	-	expression tag	UNP O94925
D	549	HIS	-	expression tag	UNP O94925
D	550	MET	-	expression tag	UNP O94925

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Na 3 3	0	0
2	D	2	Total Na 2 2	0	0
2	C	1	Total Na 1 1	0	0

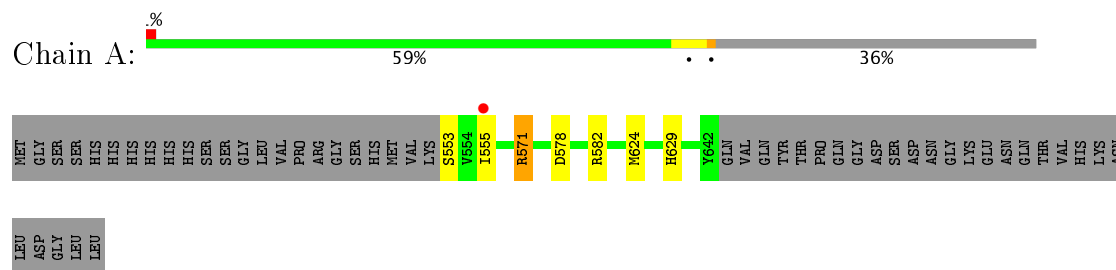
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	151	Total O 151 151	0	0
3	B	166	Total O 166 166	0	0
3	C	158	Total O 158 158	0	0
3	D	161	Total O 161 161	0	0

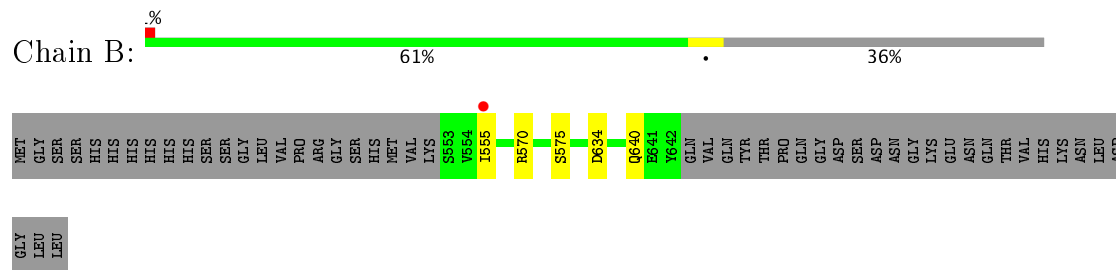
3 Residue-property plots [i](#)

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.

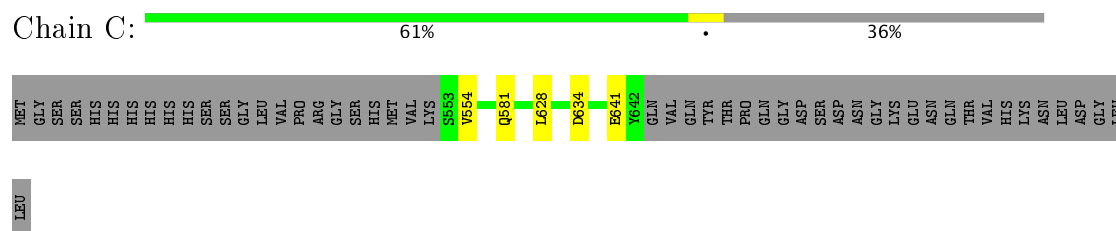
- Molecule 1: Glutaminase kidney isoform, mitochondrial



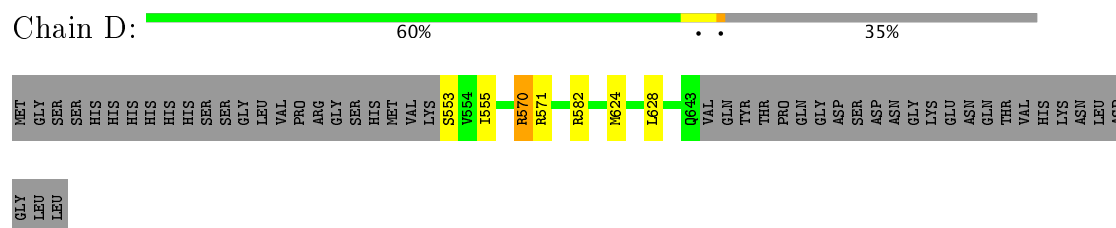
- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.49 Å 47.18 Å 115.70 Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	46.10 – 1.72 63.85 – 1.72	Depositor EDS
% Data completeness (in resolution range)	93.6 (46.10-1.72) 93.1 (63.85-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.72 Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.183 , 0.222 0.181 , 0.218	Depositor DCC
R_{free} test set	4285 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3582	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.71 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0579e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	0.93	1/748 (0.1%)	0.91	4/1013 (0.4%)
1	B	0.88	0/754	0.89	2/1021 (0.2%)
1	C	0.88	0/756	0.88	1/1024 (0.1%)
1	D	0.91	0/757	0.95	5/1025 (0.5%)
All	All	0.90	1/3015 (0.0%)	0.91	12/4083 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	ARG	CZ-NH1	5.23	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	624	MET	CG-SD-CE	-7.01	88.99	100.20
1	B	634	ASP	CB-CG-OD1	6.96	124.56	118.30
1	D	570	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	634	ASP	CB-CG-OD1	6.71	124.33	118.30
1	D	570	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	582	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	582	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	571	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	571	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	624	MET	CG-SD-CE	-5.10	92.04	100.20
1	B	570	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	578	ASP	CB-CG-OD1	5.04	122.84	118.30

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	730	0	700	5	0
1	B	733	0	707	3	0
1	C	738	0	710	2	0
1	D	739	0	708	2	0
2	A	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	151	0	0	3	1
3	B	166	0	0	3	1
3	C	158	0	0	0	0
3	D	161	0	0	1	0
All	All	3582	0	2825	11	1

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 2.

All (11) 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:555:ILE:HD12	3:B:706:HOH:O	1.45	1.17
1:B:575:SER:OG	3:B:701:HOH:O	2.16	0.60
1:D:553:SER:OG	1:D:555:ILE:HG22	2.03	0.59
1:A:629:HIS:HD2	3:A:913:HOH:O	1.87	0.57
1:D:570:ARG:HD3	3:D:862:HOH:O	2.09	0.53
1:B:640[A]:GLN:OE1	3:B:702:HOH:O	2.20	0.48
1:A:571:ARG:NH2	3:A:802:HOH:O	2.27	0.47
1:A:553:SER:N	3:A:806:HOH:O	2.49	0.45
1:A:555:ILE:HB	1:B:555:ILE:HG13	1.99	0.45
1:C:554:VAL:HG23	1:C:581:GLN:HG3	2.02	0.41
1:C:641:GLU:O	1:C:641:GLU:HG2	2.19	0.41

All (1) 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)
3:A:852:HOH:O	3:B:721:HOH:O[2_457]	2.14	0.06

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	89/140 (64%)	88 (99%)	1 (1%)	0	100	100
1	B	90/140 (64%)	89 (99%)	1 (1%)	0	100	100
1	C	90/140 (64%)	88 (98%)	2 (2%)	0	100	100
1	D	90/140 (64%)	89 (99%)	1 (1%)	0	100	100
All	All	359/560 (64%)	354 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	77/120 (64%)	77 (100%)	0	100	100
1	B	77/120 (64%)	77 (100%)	0	100	100
1	C	78/120 (65%)	76 (97%)	2 (3%)	51	30
1	D	78/120 (65%)	77 (99%)	1 (1%)	73	60
All	All	310/480 (65%)	307 (99%)	3 (1%)	87	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	628[A]	LEU
1	C	628[B]	LEU
1	D	628	LEU

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 ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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	90/140 (64%)	-0.15	1 (1%) 80 84	23, 29, 43, 57	0
1	B	90/140 (64%)	-0.10	1 (1%) 80 84	24, 31, 42, 47	0
1	C	90/140 (64%)	-0.13	0 100 100	23, 31, 41, 64	0
1	D	91/140 (65%)	-0.11	0 100 100	22, 29, 43, 77	1 (1%)
All	All	361/560 (64%)	-0.12	2 (0%) 89 92	22, 30, 43, 77	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	555	ILE	2.9
1	A	555	ILE	2.3

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	NA	A	702	1/1	0.68	0.36	-	81,81,81,81	0
2	NA	D	702	1/1	0.95	0.17	-	47,47,47,47	0
2	NA	A	701	1/1	0.95	0.05	-	41,41,41,41	0
2	NA	C	701	1/1	0.81	0.07	-	46,46,46,46	0
2	NA	A	703	1/1	0.90	0.14	-	48,48,48,48	0
2	NA	D	701	1/1	0.93	0.05	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.