



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 09:42 AM EDT

PDB ID : 3GJC
Title : Crystal Structure of the E290S mutant of LeuT with bound OG
Authors : Winther, A.M.L.; Quick, M.; Javitch, J.A.; Nissen, P.
Deposited on : unknown
Resolution : 2.80 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

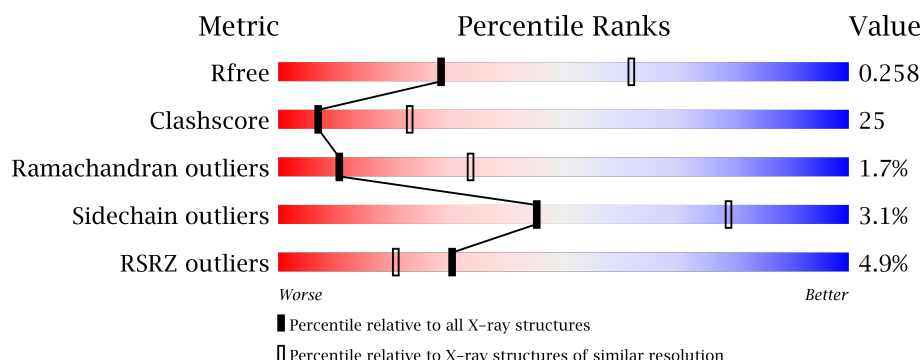
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	513	<div> <div>6%</div> <div>57%</div> <div>38%</div> <div>• •</div> </div>
1	B	513	<div> <div>4%</div> <div>58%</div> <div>37%</div> <div>• •</div> </div>

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
2	NA	A	514	-	-	-	X
2	NA	B	514	-	-	-	X
4	BOG	A	702	-	-	-	X
4	BOG	A	704	-	-	-	X
4	BOG	B	701	-	-	-	X
4	BOG	B	702	-	-	-	X
4	BOG	B	704	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8106 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 Transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3947	2678	615	643	11			
1	B	498	Total	C	N	O	S	0	0	0
			3947	2678	615	643	11			

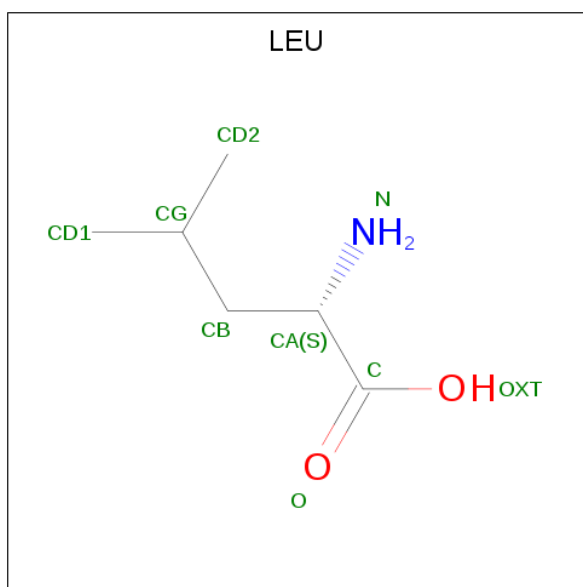
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	SER	GLU	ENGINEERED	UNP O67854
B	290	SER	GLU	ENGINEERED	UNP O67854

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

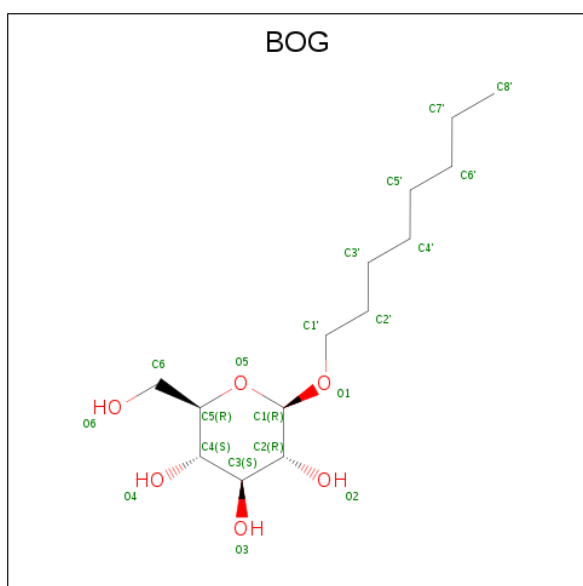
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: C₆H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

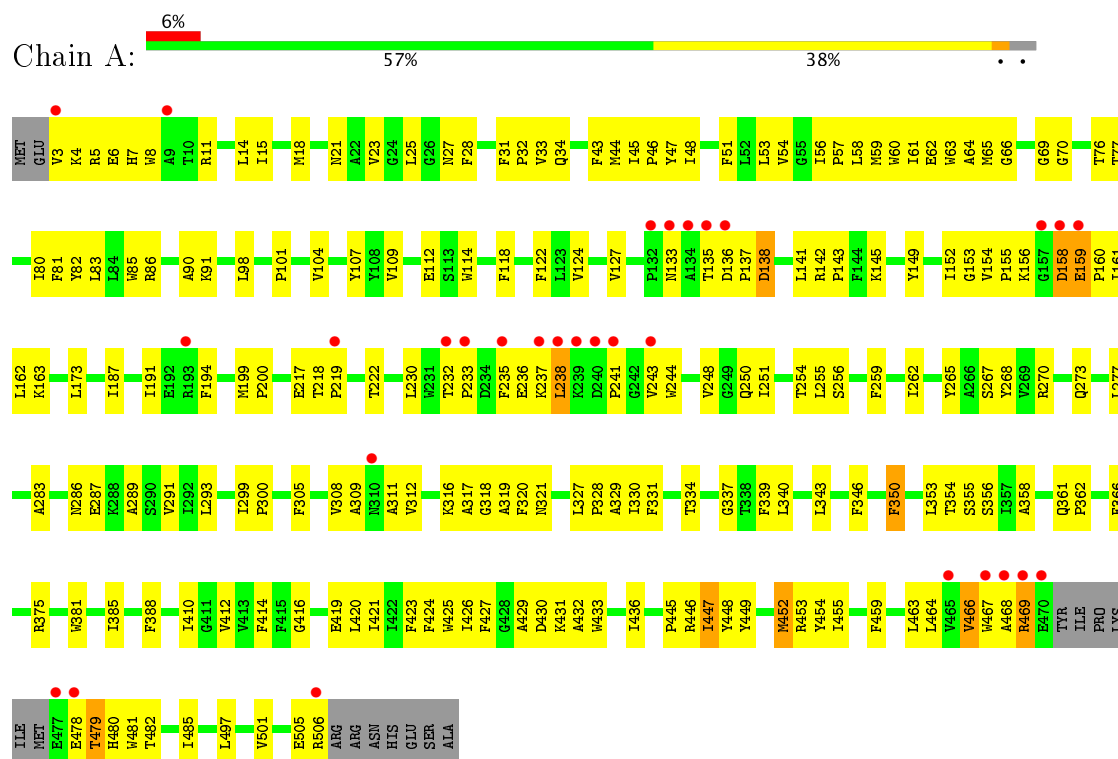
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	12	Total	O	0	0
			12	12		

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 ($\text{RSRZ} > 2$). 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: Transporter



E478	T479	H480	W481	T482	I485	L497	V501	E505	R506	ARG	ASN	HIS	GLU	SER	ALA	D401	I410	G411	V412	W413	F414	F415	G416	E419	L420	I421	I422	F423	F424	W425	I426	F427	G428	A429	D430	K431	A432	W433	I436	P445	R446	I447	Y448	Y449	Y450	V451	W452	R453	Y454	I455	T456	P457	A458	P459	I463	I464	V465	V466	W467	A468	R469	E470	TYR	ILE	PRO	LYS	ILE	MET	E477	I288	A289	S290	V291	L292	L293	I299	P300	F305	V308	A309	M310	A311	V312	K316	A317	G318	A319	F320	M321	L327	P328	A329	I330	F331	T334	G337	T338	F339	L340	L343	F346	F350	L353	T354	S355	A358	Q361	P362	F366	R375	W381	I385
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.79Å 93.51Å 87.46Å 90.00° 94.22° 90.00°	Depositor
Resolution (Å)	29.20 – 2.80 29.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.20-2.80) 97.9 (29.20-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.267 0.216 , 0.258	Depositor DCC
R_{free} test set	1032 reflections (3.17%)	DCC
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 24.22 % 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 3.9959e-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, BOG

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	0.31	0/4071	0.47	0/5547
1	B	0.32	0/4071	0.47	0/5547
All	All	0.31	0/8142	0.47	0/11094

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	3947	0	4040	216	0
1	B	3947	0	4040	207	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	9	0	10	1	0
3	B	9	0	10	1	0
4	A	80	0	112	7	0
4	B	80	0	112	6	0
5	A	20	0	0	3	0
5	B	12	0	0	3	0
All	All	8106	0	8324	418	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 25.

The worst 5 of 418 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:59:MET:CE	1:B:283:ALA:HB2	1.77	1.15
1:A:59:MET:CE	1:A:283:ALA:HB2	1.77	1.14
1:A:83:LEU:HA	1:A:86:ARG:HH12	1.12	1.12
1:B:83:LEU:HA	1:B:86:ARG:HH12	1.11	1.09
1:B:59:MET:HE1	1:B:283:ALA:CB	1.88	1.03

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	494/513 (96%)	448 (91%)	38 (8%)	8 (2%)	11	36
1	B	494/513 (96%)	446 (90%)	39 (8%)	9 (2%)	10	32
All	All	988/1026 (96%)	894 (90%)	77 (8%)	17 (2%)	11	34

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	THR
1	A	238	LEU
1	A	446	ARG
1	B	4	LYS
1	B	5	ARG

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	401/415 (97%)	388 (97%)	13 (3%)	44	78
1	B	401/415 (97%)	389 (97%)	12 (3%)	46	80
All	All	802/830 (97%)	777 (97%)	25 (3%)	45	79

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	MET
1	B	138	ASP
1	B	452	MET
1	A	469	ARG
1	B	156	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	HIS
1	B	7	HIS
1	B	333	GLN
1	A	361	GLN
1	B	321	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	LEU	A	515	-	4,8,8	0.14	0	5,10,10	0.32	0
4	BOG	A	701	-	20,20,20	0.53	0	25,25,25	1.12	1 (4%)
4	BOG	A	702	-	20,20,20	0.73	0	25,25,25	1.86	6 (24%)
4	BOG	A	703	-	20,20,20	0.73	0	25,25,25	1.45	5 (20%)
4	BOG	A	704	-	20,20,20	0.68	0	25,25,25	1.27	1 (4%)
3	LEU	B	515	-	4,8,8	0.17	0	5,10,10	0.26	0
4	BOG	B	701	-	20,20,20	0.68	0	25,25,25	1.42	5 (20%)
4	BOG	B	702	-	20,20,20	0.72	0	25,25,25	1.64	5 (20%)
4	BOG	B	703	-	20,20,20	0.70	0	25,25,25	1.49	5 (20%)
4	BOG	B	704	-	20,20,20	0.66	0	25,25,25	1.21	3 (12%)

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	LEU	A	515	-	-	0/4/8/8	0/0/0/0
4	BOG	A	701	-	-	0/11/31/31	0/1/1/1
4	BOG	A	702	-	-	0/11/31/31	0/1/1/1
4	BOG	A	703	-	-	0/11/31/31	0/1/1/1
4	BOG	A	704	-	-	0/11/31/31	0/1/1/1
3	LEU	B	515	-	-	0/4/8/8	0/0/0/0
4	BOG	B	701	-	-	0/11/31/31	0/1/1/1
4	BOG	B	702	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BOG	B	703	-	-	0/11/31/31	0/1/1/1
4	BOG	B	704	-	-	0/11/31/31	0/1/1/1

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	BOG	O5-C5-C4	2.07	113.47	109.66
4	B	704	BOG	O5-C5-C6	2.09	111.41	106.41
4	B	703	BOG	C3-C4-C5	2.09	113.89	110.22
4	A	702	BOG	C3-C4-C5	2.10	113.92	110.22
4	A	702	BOG	O5-C1-O1	2.12	115.06	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	515	LEU	1	0
4	A	701	BOG	3	0
4	A	702	BOG	2	0
4	A	704	BOG	2	0
3	B	515	LEU	1	0
4	B	701	BOG	2	0
4	B	702	BOG	1	0
4	B	704	BOG	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	498/513 (97%)	-0.02	30 (6%) 23 14	24, 47, 106, 156	0
1	B	498/513 (97%)	-0.20	19 (3%) 41 30	21, 43, 103, 157	0
All	All	996/1026 (97%)	-0.11	49 (4%) 30 20	21, 45, 105, 157	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	5.0
1	A	135	THR	4.9
1	B	134	ALA	4.8
1	B	135	THR	4.6
1	A	478	GLU	4.6

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
4	BOG	B	701	20/20	0.73	0.66	7.52	35,127,170,170	0
4	BOG	A	704	20/20	0.69	0.36	6.98	41,114,138,138	0
2	NA	A	514	1/1	0.80	0.44	6.19	59,59,59,59	0
2	NA	B	514	1/1	0.97	0.28	5.31	36,36,36,36	0
4	BOG	A	702	20/20	0.85	0.32	2.89	42,78,101,103	0
4	BOG	B	704	20/20	0.78	0.29	2.69	37,90,157,166	0
4	BOG	B	702	20/20	0.92	0.27	2.60	44,75,116,117	0
4	BOG	A	701	20/20	0.83	0.37	1.81	37,78,90,102	0
4	BOG	A	703	20/20	0.79	0.34	1.66	30,96,164,166	0
4	BOG	B	703	20/20	0.85	0.31	0.73	23,122,157,168	0
3	LEU	A	515	9/9	0.96	0.23	0.42	17,30,57,83	0
3	LEU	B	515	9/9	0.97	0.17	-0.61	20,24,37,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.