



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 12:54 PM BST

PDB ID : 3V8F
Title : Crystal structure of crosslinked GltPh V216C-M385C mutant
Authors : Verdon, G.; Boudker, O.
Deposited on : 2011-12-22
Resolution : 3.80 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

<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 : 2.14.4.dev1
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) : 2.14.4.dev1

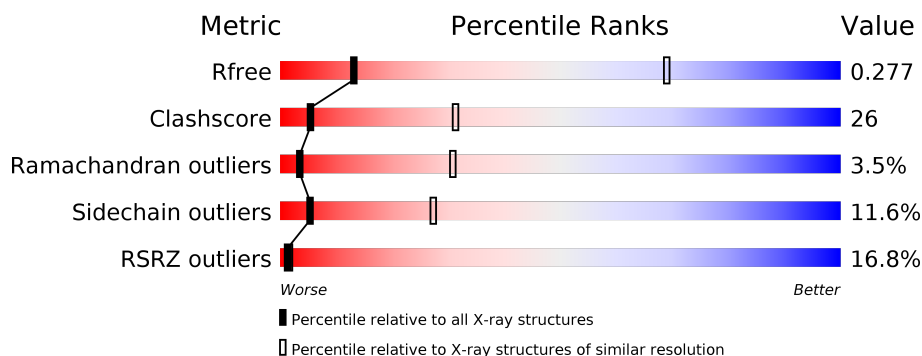
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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	422	<div> <div>24%</div> <div>48%</div> <div>43%</div> <div>6%</div> </div>
1	B	422	<div> <div>15%</div> <div>50%</div> <div>41%</div> <div>6%</div> </div>
1	C	422	<div> <div>10%</div> <div>48%</div> <div>42%</div> <div>6%</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	ASP	C	901	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9155 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 sodium-coupled L-aspartate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3038	1999	490	532	17			
1	B	411	Total	C	N	O	S	0	0	0
			3043	2002	491	533	17			
1	C	410	Total	C	N	O	S	0	0	0
			3038	1999	490	532	17			

There are 45 discrepancies between the modelled and reference sequences:

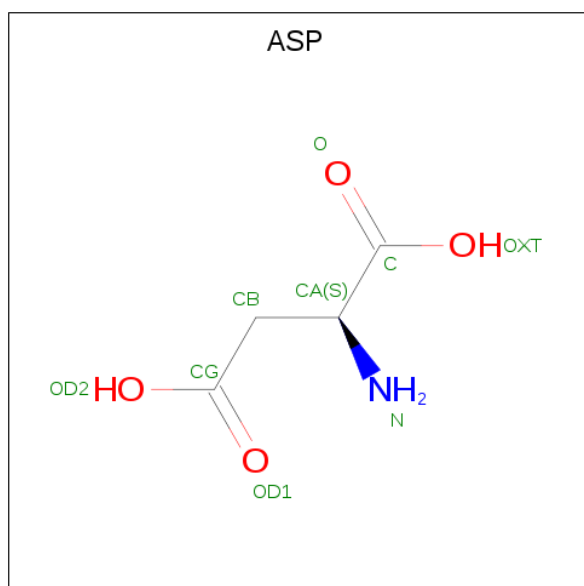
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	216	CYS	VAL	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	321	ALA	CYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	385	CYS	MET	engineered mutation	UNP O59010
A	418	THR	-	EXPRESSION TAG	UNP O59010
A	419	LEU	-	EXPRESSION TAG	UNP O59010
A	420	VAL	-	EXPRESSION TAG	UNP O59010
A	421	PRO	-	EXPRESSION TAG	UNP O59010
A	422	ARG	-	EXPRESSION TAG	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	216	CYS	VAL	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	321	ALA	CYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	368	HIS	GLU	engineered mutation	UNP O59010
B	385	CYS	MET	engineered mutation	UNP O59010
B	418	THR	-	EXPRESSION TAG	UNP O59010
B	419	LEU	-	EXPRESSION TAG	UNP O59010
B	420	VAL	-	EXPRESSION TAG	UNP O59010
B	421	PRO	-	EXPRESSION TAG	UNP O59010
B	422	ARG	-	EXPRESSION TAG	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	216	CYS	VAL	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	321	ALA	CYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	385	CYS	MET	engineered mutation	UNP O59010
C	418	THR	-	EXPRESSION TAG	UNP O59010
C	419	LEU	-	EXPRESSION TAG	UNP O59010
C	420	VAL	-	EXPRESSION TAG	UNP O59010
C	421	PRO	-	EXPRESSION TAG	UNP O59010
C	422	ARG	-	EXPRESSION TAG	UNP O59010

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



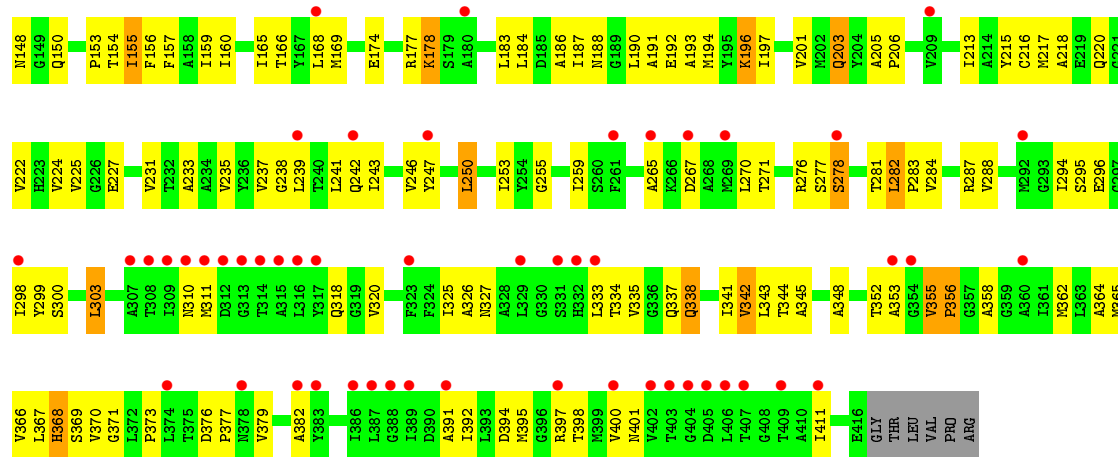
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 4 1 4	0	0
2	B	1	Total C N O 9 4 1 4	0	0
2	C	1	Total C N O 9 4 1 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

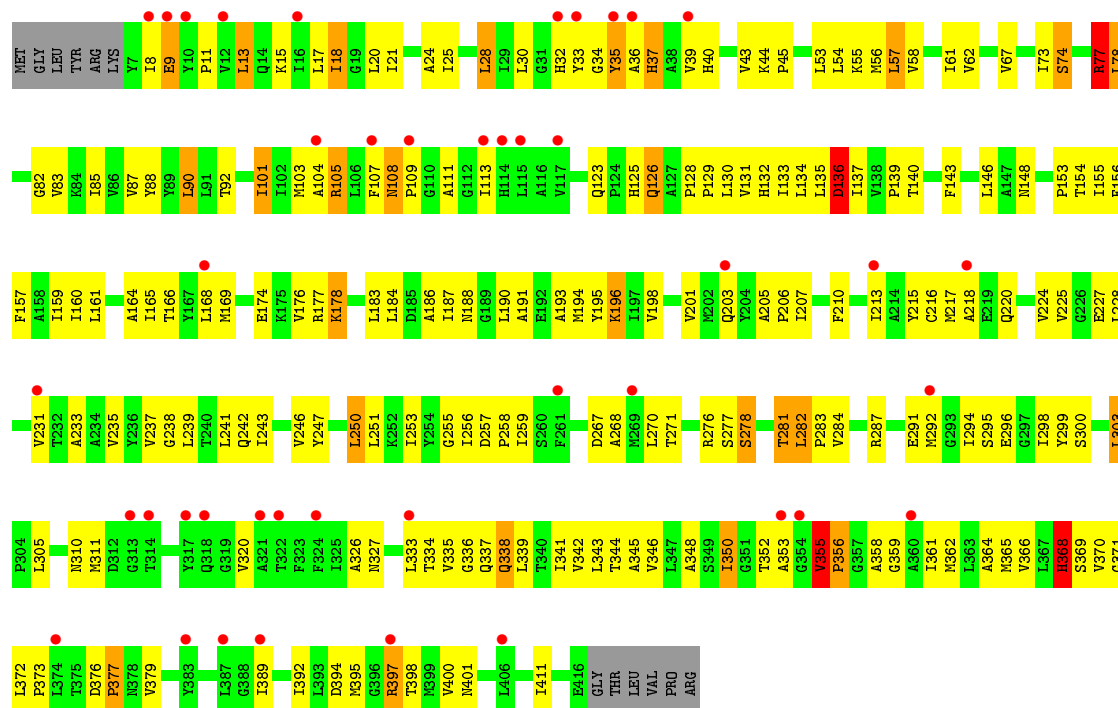
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0
3	A	2	Total Na 2 2	0	0
3	C	2	Total Na 2 2	0	0

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Hg 1 1	0	0
4	A	1	Total Hg 1 1	0	0
4	C	1	Total Hg 1 1	0	0



• Molecule 1: sodium-coupled L-aspartate transporter



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.30Å 199.81Å 111.25Å 90.00° 117.08° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 96.81 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.80) 99.5 (96.81-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 3.78Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.243 , 0.255 0.254 , 0.277	Depositor DCC
R_{free} test set	1222 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	152.4	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 238.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9155	wwPDB-VP
Average B, all atoms (Å ²)	247.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: NA, HG

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	0.53	0/3098	0.73	0/4227
1	B	0.66	0/3103	0.80	1/4234 (0.0%)
1	C	0.69	1/3098 (0.0%)	0.84	5/4227 (0.1%)
All	All	0.63	1/9299 (0.0%)	0.79	6/12688 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	ASP	CB-CG	5.03	1.62	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ARG	NE-CZ-NH1	-8.81	115.89	120.30
1	C	77	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	C	136	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	53	LEU	CA-CB-CG	-5.91	101.71	115.30
1	C	56	MET	CB-CG-SD	-5.72	95.25	112.40

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	3038	0	3204	166	0
1	B	3043	0	3206	171	0
1	C	3038	0	3204	167	0
2	A	9	0	3	2	0
2	B	9	0	3	2	0
2	C	9	0	3	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	9155	0	9623	491	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 26.

The worst 5 of 491 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:C:335:VAL:HA	1:C:338:GLN:HB2	1.44	0.97
1:A:335:VAL:HA	1:A:338:GLN:HB2	1.48	0.96
1:B:231:VAL:O	1:B:235:VAL:HG23	1.69	0.93
1:C:231:VAL:O	1:C:235:VAL:HG23	1.69	0.92
1:B:335:VAL:HA	1:B:338:GLN:HB2	1.52	0.91

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	408/422 (97%)	329 (81%)	66 (16%)	13 (3%)	4 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	409/422 (97%)	328 (80%)	67 (16%)	14 (3%)	3	31
1	C	408/422 (97%)	322 (79%)	70 (17%)	16 (4%)	3	28
All	All	1225/1266 (97%)	979 (80%)	203 (17%)	43 (4%)	3	31

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	PRO
1	B	356	PRO
1	C	356	PRO
1	B	7	TYR
1	B	310	ASN

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	319/329 (97%)	285 (89%)	34 (11%)	6	30
1	B	319/329 (97%)	280 (88%)	39 (12%)	5	25
1	C	319/329 (97%)	281 (88%)	38 (12%)	5	26
All	All	957/987 (97%)	846 (88%)	111 (12%)	5	27

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	HIS
1	B	259	ILE
1	C	303	LEU
1	B	126	GLN
1	B	155	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	ASN
1	C	132	HIS
1	B	132	HIS
1	A	108	ASN
1	C	108	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
2	ASP	B	901	-	2,8,8	1.04	0	1,10,10	0.52	0
2	ASP	A	901	-	2,8,8	1.00	0	1,10,10	0.36	0
2	ASP	C	901	-	2,8,8	0.94	0	1,10,10	0.71	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
2	ASP	B	901	-	-	1/2/8/8	-
2	ASP	A	901	-	-	0/2/8/8	-
2	ASP	C	901	-	-	1/2/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	ASP	N-CA-CB-CG
2	C	901	ASP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ASP	2	0
2	A	901	ASP	2	0
2	C	901	ASP	4	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	410/422 (97%)	1.15	100 (24%) 0 0	164, 286, 403, 467	0
1	B	411/422 (97%)	0.78	65 (15%) 2 2	135, 215, 334, 372	0
1	C	410/422 (97%)	0.64	42 (10%) 6 6	132, 219, 316, 424	0
All	All	1231/1266 (97%)	0.85	207 (16%) 1 2	132, 237, 359, 467	0

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	TYR	9.5
1	A	115	LEU	8.2
1	A	313	GLY	7.2
1	A	261	PHE	7.2
1	A	247	TYR	6.6

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 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
4	HG	A	904	1/1	0.89	0.29	312,312,312,312	1
2	ASP	A	901	9/9	0.89	0.89	253,255,264,269	0
2	ASP	C	901	9/9	0.91	0.52	178,184,191,191	0
3	NA	B	903	1/1	0.92	0.29	184,184,184,184	0
2	ASP	B	901	9/9	0.93	0.68	173,178,187,190	0
3	NA	C	903	1/1	0.93	0.17	178,178,178,178	0
3	NA	A	903	1/1	0.95	0.27	258,258,258,258	0
4	HG	B	904	1/1	0.96	0.09	248,248,248,248	1
3	NA	C	902	1/1	0.97	0.41	183,183,183,183	0
4	HG	C	904	1/1	0.97	0.14	284,284,284,284	1
3	NA	A	902	1/1	0.99	0.61	275,275,275,275	0
3	NA	B	902	1/1	0.99	1.19	194,194,194,194	0

6.5 Other polymers [i](#)

There are no such residues in this entry.