



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:15 PM BST

PDB ID : 6JUD
Title : Radiation damage in *Aspergillus oryzae* pro-tyrosinase oxygen-bound C92A/H103F mutant
Authors : Fujieda, N.; Umakoshi, K.; Nishikawa, Y.; Kurisu, G.; Itoh, S.
Deposited on : 2019-04-13
Resolution : 1.56 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

<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 : 2.13.1
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) : 2.13.1

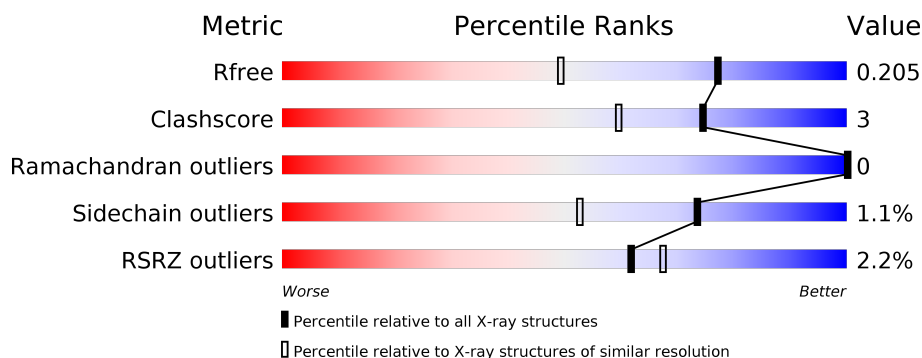
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	620	 2% 79% 7% 14%
1	B	620	 2% 82% 7% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9202 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	1	0
			4175	2701	708	754	12			
1	B	551	Total	C	N	O	S	0	0	0
			4317	2789	736	780	12			

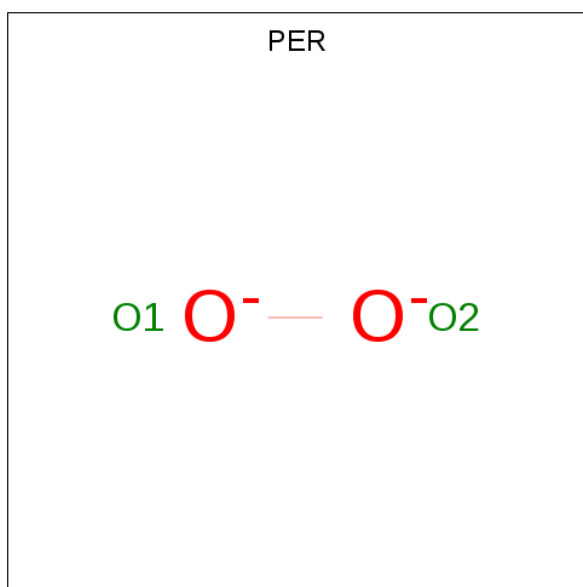
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A1S9DK56
A	-2	PRO	-	expression tag	UNP A0A1S9DK56
A	-1	GLY	-	expression tag	UNP A0A1S9DK56
A	0	GLY	-	expression tag	UNP A0A1S9DK56
A	1	SER	-	expression tag	UNP A0A1S9DK56
A	92	ALA	CYS	engineered mutation	UNP A0A1S9DK56
A	103	PHE	HIS	engineered mutation	UNP A0A1S9DK56
B	-3	GLY	-	expression tag	UNP A0A1S9DK56
B	-2	PRO	-	expression tag	UNP A0A1S9DK56
B	-1	GLY	-	expression tag	UNP A0A1S9DK56
B	0	GLY	-	expression tag	UNP A0A1S9DK56
B	1	SER	-	expression tag	UNP A0A1S9DK56
B	92	ALA	CYS	engineered mutation	UNP A0A1S9DK56
B	103	PHE	HIS	engineered mutation	UNP A0A1S9DK56

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		

- Molecule 3 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	335	Total O 343 343	0	8
4	B	357	Total O 361 361	0	4

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Chain A:

29% 7% 14%

GLY PRO GLY GLY S1 P2 L16 L27 S31 A14 GLY SER ASN R36 G68 W71 W74 D75 G79 GLN LYS ASP SER LYS GLY ASN PRO T89 F99 P100 Y106 A152 R153 HIS GLY HIS ASP ASN THR GLN D152 K176 G181 Q182 P183 C184 K195 Q196 T211 T212 SER GLN LYS THR GLU GLU HIS GLY TRP PHE D224 T233 E240 N241 Y267 Q268 N269 L270 ASP GLY THR D274 R301 P304 LYS LYS GLU GLU THR PRO LYS ASN ASN GLU GLN A317 H328 N333 F338 D347 H355 T356 P360 A363 F368 K400 D403 P406 C411 T414 R415 R421 S422 D423 D440 A441 S442 G453 GLN ARG THR LYS VAL TYR LYS ASP PHE GLY GLU E466 K496 R502 F511 G515 SER LEU GLU ASP SER CYS ASP CYS A526 T543 E573 T583 GLY THR PHE TYR ASP ALA PRO ARG GLY SER ASP D598 D611 A616

Chain B:

29%

82%

7%

11%

0.15
0.10
0.05
0.00

0.00 0.05 0.10 0.15

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300

G-3
P-2
G-1
G0
D11
P12
K13
H14
Q29
THR
SER
ALA
GLY
SER
ASN
R36
Q81
LVS
ASP
SER
LYS
GLY
ASN
P88
T89
Y97
N136
W146
R153
HIS
GLY
HIS
ASP
ASN
THR
GLN
GLY
D162
P167
G184
T212
SER
GLN
LYS
THR
GLU
HIS
GLY
THR

S222
F223
T233
E240
N241
Y267
G272
F284
T288
D303
ASP
LYS
LYS
GLU
GLU
THR
GLN
PRO
LYS
ASN
ASN
GLU
GLN
A317
P318
K319
H328
V331
F338
K349
H355
S358
V359
P360
A363
F368
S396
R405
R409
F410
P415
F420
D440
ALA
SER
R443
V459
D462
K496
Q504
F513
S514
GLY
SER
LEU
GLU
ASP
SER
ASN
CYS
ASP
CYS
GLU
ALA
GLN
GLN
GLN
GLY
GLY
V533
R542
L543
H546
K550
T563
D589
ALA
PRO
ALA
ARG
GLY
GLY
SER
D597
D598
Y599
T611

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.41Å 118.29Å 79.55Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	30.00 – 1.56 35.58 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.56) 99.6 (35.58-1.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.56Å)	Xtriage
Refinement program	SHELXL 2017/1	Depositor
R, R_{free}	0.170 , 0.229 0.151 , 0.205	Depositor DCC
R_{free} test set	7125 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: PER, CU

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	0/4304	0.76	4/5868 (0.1%)
1	B	0.31	0/4448	0.77	2/6069 (0.0%)
All	All	0.31	0/8752	0.76	6/11937 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	B	405	ARG	CD-NE-CZ	6.48	132.67	123.60
1	A	106	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	106	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	36	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	301	ARG	NE-CZ-NH2	5.28	122.94	120.30

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	4175	0	3846	25	0
1	B	4317	0	3948	27	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	B	2	0	0	0	0
4	A	343	0	0	2	0
4	B	361	0	0	3	0
All	All	9202	0	7794	52	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 3.

All (52) 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:27:LEU:O	1:A:31:SER:HB2	1.64	0.98
1:A:176:LYS:HE3	1:A:186:GLN:OE1	1.82	0.79
1:B:319:LYS:HE2	1:B:599:TYR:HE1	1.48	0.77
1:B:319:LYS:HE2	1:B:599:TYR:CE1	2.20	0.77
1:A:496:LYS:HE3	1:A:611:ASP:OD2	1.88	0.73
1:A:176:LYS:CE	1:A:186:GLN:OE1	2.38	0.71
1:B:36:ARG:HG2	1:B:36:ARG:O	1.91	0.70
1:B:319:LYS:HD2	1:B:319:LYS:O	1.92	0.69
1:B:496:LYS:HE3	1:B:611:ASP:OD1	1.95	0.66
1:B:36:ARG:O	1:B:36:ARG:CG	2.49	0.60
1:B:284:PHE:CE1	1:B:288:THR:HG21	2.37	0.59
1:A:240:GLU:O	1:A:241:ASN:CB	2.49	0.58
1:A:240:GLU:O	1:A:241:ASN:HB3	2.03	0.57
1:B:153:ARG:C	4:B:801:HOH:O	2.41	0.57
1:B:240:GLU:O	1:B:241:ASN:CB	2.53	0.56
1:B:319:LYS:CD	1:B:319:LYS:O	2.55	0.55
1:B:546:HIS:CE1	1:B:550:LYS:HE3	2.42	0.54
1:B:11:ASP:OD1	1:B:12:PRO:HD2	2.09	0.53
1:A:1:SER:HA	1:A:2:PRO:C	2.29	0.52
1:A:573:GLU:OE1	1:A:573:GLU:N	2.39	0.51
1:A:359:VAL:HB	1:A:360:PRO:HD3	1.93	0.50
1:B:359:VAL:HG21	1:B:514:SER:HA	1.92	0.50
1:A:347:ASP:CB	4:B:1024:HOH:O	2.59	0.50
1:A:74:TRP:CE3	1:A:75:ASP:HB2	2.46	0.50
1:A:267:TYR:OH	1:A:543:LEU:HB3	2.13	0.49
1:A:233:THR:HA	1:A:355:HIS:CE1	2.48	0.49
1:A:68:GLY:HA2	1:A:71[B]:TRP:CZ3	2.48	0.48
1:B:358:SER:OG	1:B:360:PRO:HD2	2.12	0.48
1:B:81:GLN:C	1:B:89:THR:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:HB2	1:A:511:PHE:CD2	2.49	0.47
1:B:14:HIS:HE1	1:B:136:ASN:OD1	1.97	0.47
1:B:542:ARG:C	1:B:542:ARG:HD3	2.33	0.47
1:A:152:ALA:O	1:A:153:ARG:O	2.33	0.46
1:B:363:ALA:HA	1:B:368:PHE:CG	2.50	0.46
1:B:583:THR:HG1	1:B:597:ASP:N	2.12	0.46
1:A:269:ASN:HB2	4:A:964:HOH:O	2.16	0.45
1:A:403:ASP:OD1	1:A:421:ARG:HD2	2.17	0.45
1:A:333:ASN:HB2	1:A:511:PHE:CG	2.53	0.44
1:A:27:LEU:O	1:A:31:SER:CB	2.52	0.42
1:A:411:CYS:O	1:A:415:ARG:N	2.52	0.42
1:B:349:LYS:HD3	4:B:1061:HOH:O	2.20	0.42
1:B:233:THR:HA	1:B:355:HIS:CE1	2.54	0.41
1:B:459:VAL:O	1:B:462:ASP:HB2	2.20	0.41
1:A:16:LEU:HD11	4:A:1123:HOH:O	2.19	0.41
1:A:363:ALA:HA	1:A:368:PHE:CG	2.56	0.41
1:A:99:PHE:HB3	1:A:100:PRO:HD3	2.01	0.41
1:B:146:TRP:CD1	1:B:167:PRO:HG3	2.55	0.41
1:B:409:ARG:HB3	1:B:420:PHE:CE1	2.56	0.41
1:B:97:TYR:CD2	1:B:396:SER:HA	2.56	0.41
1:A:400:LYS:NZ	1:A:423:ASP:OD2	2.49	0.40
1:B:359:VAL:HG22	1:B:513:PHE:CE2	2.56	0.40
1:B:267:TYR:OH	1:B:543:LEU:HB3	2.21	0.40

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	514/620 (83%)	503 (98%)	11 (2%)	0	100	100
1	B	533/620 (86%)	524 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1047/1240 (84%)	1027 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	414/536 (77%)	410 (99%)	4 (1%)	76	57
1	B	425/536 (79%)	420 (99%)	5 (1%)	71	49
All	All	839/1072 (78%)	830 (99%)	9 (1%)	73	53

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	HIS
1	A	338	PHE
1	A	406	PRO
1	A	502	ARG
1	B	36	ARG
1	B	328	HIS
1	B	338	PHE
1	B	504	GLN
1	B	542	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	HIS
1	B	14	HIS

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 5 ligands modelled in this entry, 4 are 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	$\# Z > 2$
3	PER	B	703	2	0,1,1	0.00	-	-		

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 [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	533/620 (85%)	-0.13	12 (2%) 60 66	11, 19, 38, 68	0
1	B	551/620 (88%)	-0.20	12 (2%) 62 67	11, 19, 38, 54	0
All	All	1084/1240 (87%)	-0.16	24 (2%) 62 67	11, 19, 38, 68	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	ALA	4.6
1	B	223	PHE	4.2
1	A	414	THR	3.4
1	A	211	ILE	3.4
1	B	184	GLY	3.1
1	A	185	LYS	3.1
1	B	410	PHE	3.1
1	A	442	SER	3.0
1	B	272	GLY	2.9
1	A	440	ASP	2.8
1	A	181	GLY	2.8
1	B	331	VAL	2.7
1	B	-1	GLY	2.4
1	A	411	CYS	2.4
1	A	183	PRO	2.4
1	B	0	GLY	2.3
1	A	616	ALA	2.3
1	B	589	ASP	2.3
1	B	222	SER	2.2
1	B	-2	PRO	2.1
1	A	184	GLY	2.1
1	A	441	ALA	2.1
1	B	88	PRO	2.0
1	B	415	ARG	2.0

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
3	PER	B	703	2/2	0.97	0.08	21,21,21,23	2
2	CU	A	701	1/1	0.99	0.04	25,25,25,25	1
2	CU	A	702	1/1	1.00	0.09	13,13,13,13	1
2	CU	B	702	1/1	1.00	0.09	20,20,20,20	1
2	CU	B	701	1/1	1.00	0.04	18,18,18,18	1

6.5 Other polymers [i](#)

There are no such residues in this entry.