



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:17 AM GMT

PDB ID : 3HUH
Title : The structure of biphenyl-2,3-diol 1,2-dioxygenase iii-related protein from salmonella typhimurium
Authors : Fedorov, A.A.; Fedorov, E.V.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-06-14
Resolution : 1.50 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
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

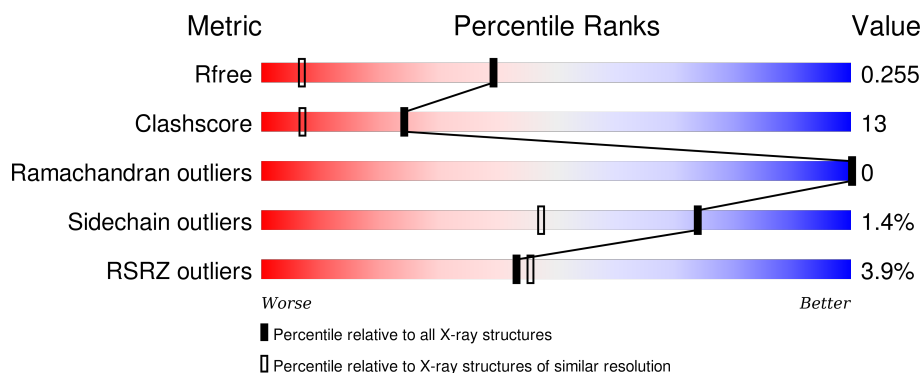
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	152	<div> <div>2%</div> <div>62% 20% 18%</div> </div>
1	B	152	<div> <div>5%</div> <div>57% 20% 22%</div> </div>
1	C	152	<div> <div>4%</div> <div>62% 16% 22%</div> </div>
1	D	152	<div> <div>2%</div> <div>56% 25% 18%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4083 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 Virulence protein STM3117.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			966	613	160	190	3			
1	B	119	Total	C	N	O	S	0	0	0
			920	584	154	180	2			
1	C	119	Total	C	N	O	S	0	0	0
			920	584	154	180	2			
1	D	124	Total	C	N	O	S	0	0	0
			966	613	160	190	3			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8ZM36
A	2	SER	-	expression tag	UNP Q8ZM36
A	3	LEU	-	expression tag	UNP Q8ZM36
A	145	GLU	-	expression tag	UNP Q8ZM36
A	146	GLY	-	expression tag	UNP Q8ZM36
A	147	HIS	-	expression tag	UNP Q8ZM36
A	148	HIS	-	expression tag	UNP Q8ZM36
A	149	HIS	-	expression tag	UNP Q8ZM36
A	150	HIS	-	expression tag	UNP Q8ZM36
A	151	HIS	-	expression tag	UNP Q8ZM36
A	152	HIS	-	expression tag	UNP Q8ZM36
B	1	MET	-	expression tag	UNP Q8ZM36
B	2	SER	-	expression tag	UNP Q8ZM36
B	3	LEU	-	expression tag	UNP Q8ZM36
B	145	GLU	-	expression tag	UNP Q8ZM36
B	146	GLY	-	expression tag	UNP Q8ZM36
B	147	HIS	-	expression tag	UNP Q8ZM36
B	148	HIS	-	expression tag	UNP Q8ZM36
B	149	HIS	-	expression tag	UNP Q8ZM36
B	150	HIS	-	expression tag	UNP Q8ZM36
B	151	HIS	-	expression tag	UNP Q8ZM36

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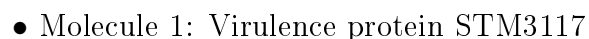
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Chain	Residue	Modelled	Actual	Comment	Reference
B	152	HIS	-	expression tag	UNP Q8ZM36
C	1	MET	-	expression tag	UNP Q8ZM36
C	2	SER	-	expression tag	UNP Q8ZM36
C	3	LEU	-	expression tag	UNP Q8ZM36
C	145	GLU	-	expression tag	UNP Q8ZM36
C	146	GLY	-	expression tag	UNP Q8ZM36
C	147	HIS	-	expression tag	UNP Q8ZM36
C	148	HIS	-	expression tag	UNP Q8ZM36
C	149	HIS	-	expression tag	UNP Q8ZM36
C	150	HIS	-	expression tag	UNP Q8ZM36
C	151	HIS	-	expression tag	UNP Q8ZM36
C	152	HIS	-	expression tag	UNP Q8ZM36
D	1	MET	-	expression tag	UNP Q8ZM36
D	2	SER	-	expression tag	UNP Q8ZM36
D	3	LEU	-	expression tag	UNP Q8ZM36
D	145	GLU	-	expression tag	UNP Q8ZM36
D	146	GLY	-	expression tag	UNP Q8ZM36
D	147	HIS	-	expression tag	UNP Q8ZM36
D	148	HIS	-	expression tag	UNP Q8ZM36
D	149	HIS	-	expression tag	UNP Q8ZM36
D	150	HIS	-	expression tag	UNP Q8ZM36
D	151	HIS	-	expression tag	UNP Q8ZM36
D	152	HIS	-	expression tag	UNP Q8ZM36

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	96	Total O 96 96	0	0
2	B	73	Total O 73 73	0	0
2	C	62	Total O 62 62	0	0
2	D	80	Total O 80 80	0	0

- Molecule 1: Virulence protein STM3117



I104	I109	S110	I111	V112	E113	G114	P115	V116	E117	R118	T119	E124	I125	M126	S127	I128	Y129	P133	N136	Y143	VAL	GLU	GLY	HIS	HIS	HIS	HIS	HIS	HIS
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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	39.90Å 138.25Å 51.41Å 90.00° 112.91° 90.00°	Depositor
Resolution (Å)	24.77 – 1.50 36.79 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (24.77-1.50) 95.3 (36.79-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.256 0.234 , 0.255	Depositor DCC
R_{free} test set	3924 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.5	EDS
Estimated twinning fraction	0.136 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78087 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4083	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/982	0.64	0/1332
1	B	0.31	0/934	0.62	0/1267
1	C	0.31	0/934	0.62	0/1267
1	D	0.34	0/982	0.64	0/1332
All	All	0.32	0/3832	0.63	0/5198

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 [i](#)

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	966	0	968	25	0
1	B	920	0	929	29	0
1	C	920	0	929	20	0
1	D	966	0	968	32	0
2	A	96	0	0	1	0
2	B	73	0	0	4	0
2	C	62	0	0	2	0
2	D	80	0	0	0	0
All	All	4083	0	3794	98	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 13.

All (98) 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:114:GLY:HA2	1:C:116:VAL:HG23	1.45	0.97
1:A:114:GLY:HA2	1:A:116:VAL:HG23	1.51	0.93
1:D:114:GLY:HA2	1:D:116:VAL:HG13	1.56	0.88
1:A:57:LYS:HE2	2:A:299:HOH:O	1.78	0.84
1:A:53:LYS:HE2	1:B:119:THR:HG23	1.60	0.82
1:B:44:VAL:HG21	1:B:109:ILE:HD11	1.70	0.73
1:C:128:ILE:HD13	1:C:129:TYR:N	2.05	0.71
1:B:128:ILE:HD13	1:B:129:TYR:N	2.07	0.69
1:D:25:ASP:OD2	1:D:26:HIS:HD2	1.76	0.68
1:D:128:ILE:HD13	1:D:129:TYR:N	2.10	0.67
1:A:25:ASP:OD2	1:A:26:HIS:HD2	1.78	0.66
1:B:54:GLN:HG2	1:B:56:ARG:HG2	1.78	0.64
1:B:114:GLY:HA2	1:B:116:VAL:HG13	1.81	0.63
1:A:113:GLU:OE2	1:B:77:PRO:HD3	1.99	0.63
1:C:87:ALA:H	1:C:136:ASN:ND2	1.96	0.62
1:C:25:ASP:OD2	1:C:26:HIS:HD2	1.81	0.62
1:D:117:GLU:HG3	1:D:126:MET:CE	2.30	0.62
1:D:87:ALA:H	1:D:136:ASN:ND2	1.98	0.61
1:C:53:LYS:O	1:C:56:ARG:HD3	2.00	0.61
1:A:87:ALA:H	1:A:136:ASN:ND2	1.98	0.61
1:D:117:GLU:HG3	1:D:126:MET:HE1	1.83	0.59
1:B:87:ALA:H	1:B:136:ASN:ND2	1.99	0.59
1:B:25:ASP:OD2	1:B:26:HIS:HD2	1.86	0.58
1:C:87:ALA:H	1:C:136:ASN:HD22	1.52	0.58
1:C:50:VAL:HG11	1:C:60:ILE:HD12	1.86	0.58
1:A:22:ASP:HB2	2:B:193:HOH:O	2.04	0.57
2:C:264:HOH:O	1:D:53:LYS:HE2	2.03	0.57
1:B:60:ILE:HG23	2:B:173:HOH:O	2.03	0.57
1:D:73:MET:O	1:D:73:MET:HG3	2.04	0.57
1:D:98:ASN:O	1:D:101:VAL:HG12	2.06	0.56
1:B:35:SER:O	1:B:39:ARG:HG3	2.06	0.55
1:B:45:LEU:HD21	1:B:140:ILE:CD1	2.36	0.55
1:C:92:ILE:HG12	1:D:25:ASP:HB2	1.89	0.54
1:B:45:LEU:HD21	1:B:140:ILE:HD11	1.89	0.54
1:A:104:ILE:HG23	1:A:109:ILE:HB	1.90	0.54
1:C:34:ILE:HG12	1:C:70:GLN:HB2	1.89	0.54
1:B:87:ALA:H	1:B:136:ASN:HD22	1.56	0.53
1:C:35:SER:O	1:C:39:ARG:HG3	2.08	0.53
1:A:87:ALA:H	1:A:136:ASN:HD22	1.56	0.53
1:D:61:PHE:HE2	1:D:66:ILE:HG12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:HG22	1:D:109:ILE:HD11	1.92	0.52
1:A:117:GLU:HG2	1:A:126:MET:HE1	1.90	0.52
1:A:44:VAL:CG2	1:A:109:ILE:HD11	2.40	0.51
1:B:44:VAL:CG2	1:B:109:ILE:HD11	2.38	0.51
1:B:27:LEU:HD11	1:B:66:ILE:HD12	1.93	0.51
1:A:117:GLU:HG2	1:A:126:MET:CE	2.41	0.51
1:A:20:ILE:HD13	2:B:244:HOH:O	2.09	0.50
1:D:44:VAL:CG2	1:D:109:ILE:HD11	2.41	0.50
1:B:52:PHE:O	1:B:56:ARG:HB2	2.12	0.50
1:C:60:ILE:HG23	2:C:183:HOH:O	2.12	0.50
1:D:98:ASN:O	1:D:101:VAL:CG1	2.60	0.49
1:D:111:ILE:HG12	1:D:128:ILE:HD11	1.94	0.49
1:D:119:THR:HG22	1:D:124:GLU:OE1	2.13	0.49
1:B:44:VAL:HG21	1:B:109:ILE:CD1	2.42	0.49
1:C:25:ASP:HB2	1:D:92:ILE:HG12	1.95	0.49
1:A:44:VAL:HG22	1:A:109:ILE:HD11	1.95	0.49
1:A:25:ASP:HB2	1:B:92:ILE:HG12	1.94	0.48
1:B:56:ARG:HH11	1:B:56:ARG:HG3	1.78	0.48
1:D:70:GLN:HB3	1:D:73:MET:HG2	1.96	0.48
1:A:84:PRO:O	1:B:81:ARG:HD3	2.13	0.48
1:D:104:ILE:HG23	1:D:109:ILE:HB	1.95	0.47
1:A:71:GLN:O	1:A:72:GLU:HB2	2.14	0.47
1:C:81:ARG:HD3	1:D:84:PRO:O	2.15	0.47
1:C:128:ILE:C	1:C:128:ILE:HD13	2.35	0.47
1:D:35:SER:O	1:D:39:ARG:HG3	2.14	0.47
1:D:51:THR:HA	1:D:56:ARG:O	2.15	0.47
1:C:44:VAL:CG2	1:C:109:ILE:HD11	2.44	0.47
1:B:53:LYS:HB3	1:B:54:GLN:OE1	2.16	0.46
1:C:117:GLU:HG3	1:C:126:MET:HE1	1.98	0.46
1:D:98:ASN:HA	1:D:101:VAL:HG12	1.97	0.45
1:A:111:ILE:CG2	1:A:128:ILE:HD11	2.46	0.45
1:A:51:THR:HA	1:A:56:ARG:O	2.16	0.45
1:D:87:ALA:H	1:D:136:ASN:HD22	1.65	0.45
1:B:50:VAL:HG11	1:B:60:ILE:HD12	1.99	0.45
1:C:117:GLU:HG3	1:C:126:MET:CE	2.47	0.44
1:B:128:ILE:C	1:B:128:ILE:HD13	2.38	0.44
1:D:41:TYR:CD2	1:D:45:LEU:HD12	2.53	0.44
1:C:44:VAL:HG22	1:C:109:ILE:HD11	1.99	0.44
1:D:41:TYR:HD2	1:D:45:LEU:HD12	1.83	0.44
1:D:71:GLN:O	1:D:72:GLU:HB2	2.19	0.43
1:B:39:ARG:HG2	2:B:300:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:HG12	1:C:128:ILE:HD11	2.01	0.43
1:A:39:ARG:O	1:A:43:GLU:HG3	2.19	0.43
1:D:128:ILE:C	1:D:128:ILE:HD13	2.39	0.43
1:D:40:PHE:CG	1:D:133:PRO:HD3	2.54	0.42
1:B:34:ILE:HG12	1:B:70:GLN:HB2	2.01	0.42
1:A:111:ILE:HD13	1:A:128:ILE:HD11	2.02	0.42
1:B:132:ASP:HB2	1:B:133:PRO:CD	2.50	0.42
1:A:92:ILE:HG12	1:B:25:ASP:HB2	2.02	0.42
1:D:113:GLU:OE2	1:D:118:ARG:NH2	2.53	0.41
1:D:53:LYS:O	1:D:54:GLN:HB3	2.20	0.41
1:B:61:PHE:HE2	1:B:66:ILE:HG12	1.86	0.41
1:B:45:LEU:HD23	1:B:45:LEU:HA	1.88	0.41
1:A:34:ILE:HG13	1:A:70:GLN:HB2	2.02	0.41
1:A:61:PHE:HE2	1:A:66:ILE:HG13	1.85	0.41
1:C:36:THR:HA	1:C:39:ARG:HD2	2.04	0.40
1:A:111:ILE:HG21	1:A:128:ILE:HD11	2.03	0.40
1:D:73:MET:CG	1:D:73:MET:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	122/152 (80%)	118 (97%)	4 (3%)	0	100	100
1	B	115/152 (76%)	112 (97%)	3 (3%)	0	100	100
1	C	115/152 (76%)	115 (100%)	0	0	100	100
1	D	122/152 (80%)	119 (98%)	3 (2%)	0	100	100
All	All	474/608 (78%)	464 (98%)	10 (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	109/135 (81%)	109 (100%)	0	100	100
1	B	104/135 (77%)	102 (98%)	2 (2%)	65	31
1	C	104/135 (77%)	102 (98%)	2 (2%)	65	31
1	D	109/135 (81%)	107 (98%)	2 (2%)	66	35
All	All	426/540 (79%)	420 (99%)	6 (1%)	74	47

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	69	HIS
1	B	128	ILE
1	C	69	HIS
1	C	128	ILE
1	D	69	HIS
1	D	128	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	69	HIS
1	A	136	ASN
1	B	26	HIS
1	B	55	ASN
1	B	69	HIS
1	B	136	ASN
1	C	26	HIS
1	C	55	ASN
1	C	136	ASN
1	D	26	HIS
1	D	69	HIS
1	D	136	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](#)

There are no ligands in this entry.

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 ⓘ

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	124/152 (81%)	0.29	2 (1%) 74 78	15, 20, 29, 34	0
1	B	119/152 (78%)	0.37	8 (6%) 21 21	15, 23, 35, 44	0
1	C	119/152 (78%)	0.43	6 (5%) 32 34	16, 23, 34, 43	0
1	D	124/152 (81%)	0.33	3 (2%) 62 66	15, 21, 30, 33	0
All	All	486/608 (79%)	0.36	19 (3%) 43 45	15, 22, 32, 44	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	LYS	5.5
1	D	73	MET	4.8
1	C	54	GLN	4.4
1	B	54	GLN	4.4
1	B	52	PHE	3.8
1	D	39	ARG	3.3
1	B	56	ARG	3.1
1	B	39	ARG	3.0
1	D	20	ILE	2.9
1	B	76	GLU	2.8
1	C	128	ILE	2.6
1	A	39	ARG	2.5
1	C	103	GLU	2.4
1	C	56	ARG	2.3
1	B	128	ILE	2.2
1	B	55	ASN	2.2
1	A	109	ILE	2.1
1	C	20	ILE	2.1
1	B	60	ILE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.