



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 08:46 PM UTC

PDB ID : 8QPM / pdb_00008qpm
Title : Structure of methylene-tetrahydromethanopterin reductase from Methanocaldococcus jannaschii
Authors : Gehl, M.; Demmer, U.; Ermler, U.; Shima, S.
Deposited on : 2023-10-02
Resolution : 1.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

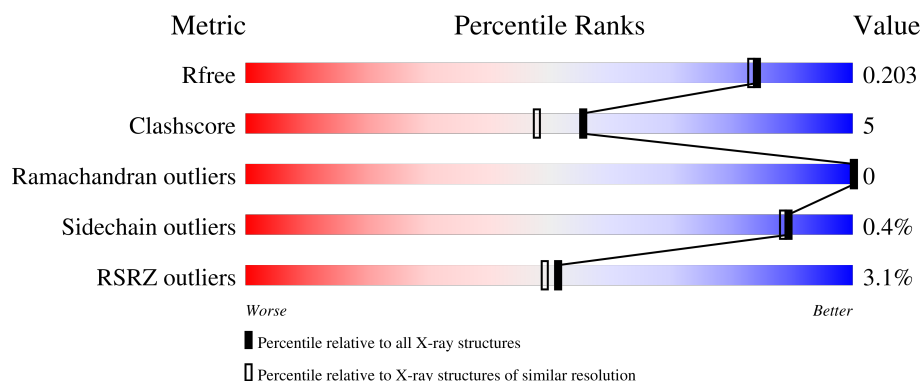
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 of 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	335	92% 6% .
1	B	335	91% 7% .
1	C	335	6% 85% 12% .
1	D	335	6% 86% 12% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20639 atoms, of which 10151 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 5,10-methylenetetrahydromethanopterin reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	H	N	O	S	0	0	0
			5006	1576	2545	409	461	15			
1	B	329	Total	C	H	N	O	S	0	0	0
			5006	1576	2545	409	461	15			
1	C	327	Total	C	H	N	O	S	0	0	0
			4977	1567	2529	407	459	15			
1	D	329	Total	C	H	N	O	S	0	0	0
			4993	1576	2532	409	461	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ALA	-	expression tag	UNP A0A832SYB5
A	333	LEU	-	expression tag	UNP A0A832SYB5
A	334	LYS	-	expression tag	UNP A0A832SYB5
A	335	GLU	-	expression tag	UNP A0A832SYB5
B	332	ALA	-	expression tag	UNP A0A832SYB5
B	333	LEU	-	expression tag	UNP A0A832SYB5
B	334	LYS	-	expression tag	UNP A0A832SYB5
B	335	GLU	-	expression tag	UNP A0A832SYB5
C	332	ALA	-	expression tag	UNP A0A832SYB5
C	333	LEU	-	expression tag	UNP A0A832SYB5
C	334	LYS	-	expression tag	UNP A0A832SYB5
C	335	GLU	-	expression tag	UNP A0A832SYB5
D	332	ALA	-	expression tag	UNP A0A832SYB5
D	333	LEU	-	expression tag	UNP A0A832SYB5
D	334	LYS	-	expression tag	UNP A0A832SYB5
D	335	GLU	-	expression tag	UNP A0A832SYB5

- Molecule 2 is water.

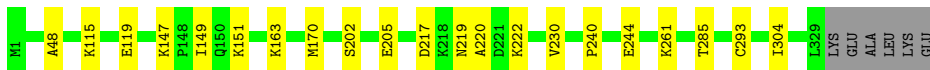
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	213	Total 213	O 213	0	0
2	B	210	Total 210	O 210	0	0
2	C	126	Total 126	O 126	0	0
2	D	108	Total 108	O 108	0	0

3 Residue-property plots

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.

- Molecule 1: 5,10-methylenetetrahydromethanopterin reductase

Chain A:  92% 6% .



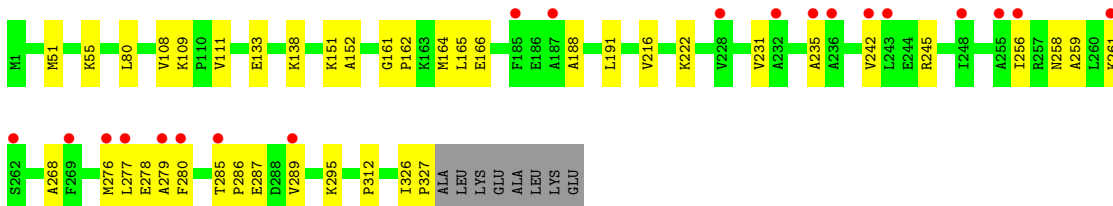
- Molecule 1: 5,10-methylenetetrahydromethanopterin reductase

Chain B:  91% 7% .



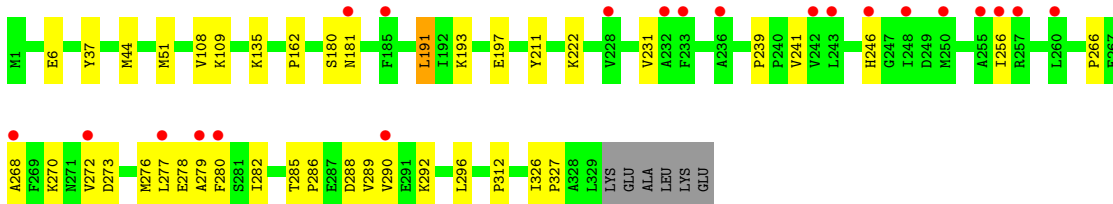
- Molecule 1: 5,10-methylenetetrahydromethanopterin reductase

Chain C:  6% 85% 12% .



- Molecule 1: 5,10-methylenetetrahydromethanopterin reductase

Chain D:  6% 86% 12% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.66Å 96.28Å 166.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 1.80 48.33 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.33-1.80) 98.8 (48.33-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.180 , 0.202 0.181 , 0.203	Depositor DCC
R_{free} test set	2003 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.407 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20639	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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

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	0.41	0/2505	0.63	2/3394 (0.1%)
1	B	0.42	0/2505	0.65	1/3394 (0.0%)
1	C	0.41	0/2492	0.61	0/3376
1	D	0.57	0/2505	0.85	2/3394 (0.1%)
All	All	0.46	0/10007	0.69	5/13558 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	GLU	CA-CB-CG	-7.02	100.05	114.10
1	D	278	GLU	N-CA-C	-6.44	104.52	112.38
1	A	149	ILE	N-CA-C	-5.98	105.89	111.45
1	A	261	LYS	CG-CD-CE	5.15	123.15	111.30
1	D	239	PRO	N-CA-CB	5.03	105.83	103.22

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	2461	2545	2545	20	0
1	B	2461	2545	2545	13	0
1	C	2448	2529	2529	36	0
1	D	2461	2532	2545	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	213	0	0	1	0
2	B	210	0	0	1	0
2	C	126	0	0	0	0
2	D	108	0	0	0	0
All	All	10488	10151	10164	91	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 5.

All (91) 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:D:282:ILE:HG22	1:D:289:VAL:HG13	1.65	0.79
1:A:151:LYS:H	1:A:151:LYS:HE2	1.51	0.76
1:A:240:PRO:O	1:A:244:GLU:HG3	1.93	0.68
1:D:285:THR:O	1:D:289:VAL:HG23	1.95	0.67
1:A:151:LYS:H	1:A:151:LYS:CE	2.09	0.65
1:C:259:ALA:HB3	1:C:268:ALA:HB2	1.79	0.65
1:C:231:VAL:HG21	1:C:277:LEU:HD23	1.81	0.63
1:A:151:LYS:H	1:A:151:LYS:CD	2.13	0.62
1:C:151:LYS:HD2	1:C:152:ALA:H	1.64	0.62
1:D:231:VAL:HG21	1:D:277:LEU:HD23	1.82	0.61
1:D:181:ASN:ND2	1:D:279:ALA:HB1	2.15	0.61
1:C:161:GLY:O	1:C:165:LEU:HD12	2.01	0.61
1:D:256:ILE:HG23	1:D:268:ALA:HB1	1.81	0.60
1:D:181:ASN:HD22	1:D:246:HIS:CE1	2.19	0.60
1:C:162:PRO:HA	1:C:165:LEU:HD13	1.86	0.58
1:D:162:PRO:HA	1:D:191:LEU:HD22	1.85	0.57
1:C:216:VAL:HG22	1:C:289:VAL:HG21	1.87	0.57
1:A:163:LYS:H	1:A:163:LYS:CD	2.19	0.56
1:C:51:MET:CE	1:D:51:MET:HE2	2.36	0.56
1:C:287:GLU:OE1	1:C:287:GLU:N	2.26	0.55
1:A:163:LYS:H	1:A:163:LYS:HE2	1.72	0.53
1:A:219:ASN:HB3	1:A:222:LYS:HG3	1.91	0.53
1:C:133:GLU:OE1	1:C:138:LYS:HE3	2.09	0.53
1:D:266:PRO:O	1:D:270:LYS:HG3	2.08	0.52
1:D:222:LYS:HE2	1:D:312:PRO:HB3	1.92	0.51
1:D:181:ASN:HD21	1:D:280:PHE:H	1.57	0.51
1:C:326:ILE:N	1:C:327:PRO:HD2	2.26	0.51
1:C:166:GLU:OE2	1:C:191:LEU:HD23	2.12	0.50
1:D:273:ASP:OD1	1:D:276:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ASP:O	1:D:292:LYS:HG3	2.12	0.49
1:A:163:LYS:H	1:A:163:LYS:HD3	1.76	0.49
1:A:163:LYS:H	1:A:163:LYS:CE	2.25	0.49
1:C:165:LEU:HD12	1:C:165:LEU:H	1.77	0.49
1:A:202:SER:O	1:A:205:GLU:HG2	2.13	0.49
1:C:235:ALA:HA	1:C:280:PHE:HE2	1.78	0.49
1:D:282:ILE:CG2	1:D:289:VAL:HG13	2.39	0.48
1:D:276:MET:O	1:D:279:ALA:O	2.32	0.48
1:D:108:VAL:O	1:D:109:LYS:C	2.58	0.47
1:C:242:VAL:HG22	1:C:245:ARG:HH21	1.79	0.47
1:C:165:LEU:CD2	1:C:188:ALA:HB1	2.45	0.46
1:D:272:VAL:HA	1:D:276:MET:SD	2.55	0.46
1:B:292:LYS:NZ	2:B:403:HOH:O	2.48	0.46
1:D:326:ILE:N	1:D:327:PRO:CD	2.79	0.46
1:A:230:VAL:HG23	2:A:423:HOH:O	2.16	0.45
1:A:293:CYS:SG	1:A:304:ILE:HD13	2.56	0.45
1:B:216:VAL:HG22	1:B:289:VAL:HG21	1.97	0.45
1:A:151:LYS:CD	1:A:151:LYS:N	2.79	0.45
1:C:51:MET:HE2	1:D:51:MET:HE2	1.96	0.45
1:C:151:LYS:HD2	1:C:152:ALA:N	2.30	0.45
1:C:295:LYS:N	1:C:295:LYS:HD3	2.32	0.45
1:A:115:LYS:NZ	1:A:119:GLU:OE1	2.50	0.45
1:C:51:MET:HE2	1:D:51:MET:CE	2.46	0.45
1:C:279:ALA:C	1:C:280:PHE:HD1	2.25	0.45
1:B:22:LEU:HD11	1:B:319:LYS:HE3	1.99	0.44
1:A:48:ALA:CB	1:B:51:MET:HE1	2.47	0.44
1:A:220:ALA:HB2	1:A:285:THR:HG23	1.99	0.44
1:C:111:VAL:HG22	1:C:164:MET:CE	2.46	0.44
1:C:55:LYS:HE2	1:C:55:LYS:HB2	1.81	0.44
1:D:135:LYS:HB3	1:D:135:LYS:HE3	1.79	0.44
1:C:287:GLU:H	1:C:287:GLU:CD	2.21	0.44
1:A:170:MET:HE2	1:A:170:MET:HB3	1.88	0.43
1:C:108:VAL:O	1:C:109:LYS:C	2.61	0.43
1:C:235:ALA:CB	1:C:276:MET:CE	2.96	0.43
1:D:6:GLU:HG3	1:D:211:TYR:OH	2.19	0.43
1:B:326:ILE:N	1:B:327:PRO:CD	2.81	0.43
1:C:278:GLU:O	1:C:278:GLU:HG3	2.18	0.43
1:C:256:ILE:HG23	1:C:268:ALA:HB1	2.00	0.43
1:C:51:MET:CE	1:D:51:MET:CE	2.96	0.43
1:C:258:ASN:HA	1:C:261:LYS:CD	2.50	0.42
1:D:37:TYR:CD1	1:D:37:TYR:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:O	1:B:298:GLU:HG3	2.20	0.42
1:C:280:PHE:CD1	1:C:280:PHE:N	2.88	0.42
1:D:286:PRO:O	1:D:290:VAL:HG23	2.20	0.42
1:A:217:ASP:O	1:A:285:THR:HA	2.19	0.42
1:B:166:GLU:O	1:B:170:MET:HG3	2.20	0.42
1:B:37:TYR:CD1	1:B:37:TYR:C	2.98	0.42
1:C:258:ASN:HA	1:C:261:LYS:HD2	2.02	0.41
1:A:202:SER:O	1:A:205:GLU:CG	2.69	0.41
1:B:202:SER:O	1:B:205:GLU:HG2	2.20	0.41
1:C:222:LYS:HE2	1:C:312:PRO:HB3	2.02	0.41
1:B:193:LYS:HD2	1:B:197:GLU:HG2	2.03	0.41
1:D:292:LYS:O	1:D:296:LEU:CD1	2.68	0.41
1:B:189:ILE:HD12	1:B:299:MET:O	2.21	0.40
1:B:265:PHE:N	1:B:266:PRO:CD	2.83	0.40
1:A:163:LYS:HD3	1:A:163:LYS:N	2.36	0.40
1:C:51:MET:HE1	1:D:51:MET:HE2	2.02	0.40
1:C:80:LEU:HB2	1:D:44:MET:HE1	2.03	0.40
1:C:280:PHE:HD1	1:C:280:PHE:N	2.19	0.40
1:C:285:THR:HB	1:C:286:PRO:HD2	2.03	0.40
1:D:193:LYS:HD2	1:D:197:GLU:HG2	2.03	0.40
1:B:108:VAL:O	1:B:109:LYS:C	2.64	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	327/335 (98%)	321 (98%)	6 (2%)	0	100	100
1	B	327/335 (98%)	320 (98%)	7 (2%)	0	100	100
1	C	325/335 (97%)	315 (97%)	10 (3%)	0	100	100
1	D	327/335 (98%)	317 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1306/1340 (98%)	1273 (98%)	33 (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	258/263 (98%)	257 (100%)	1 (0%)	89	88
1	B	258/263 (98%)	258 (100%)	0	100	100
1	C	257/263 (98%)	257 (100%)	0	100	100
1	D	258/263 (98%)	255 (99%)	3 (1%)	67	62
All	All	1031/1052 (98%)	1027 (100%)	4 (0%)	89	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LYS
1	D	180	SER
1	D	191	LEU
1	D	241	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	178	ASN
1	C	181	ASN
1	D	181	ASN
1	D	246	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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 [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	329/335 (98%)	-1.08	0	100 100	27, 41, 64, 87	0
1	B	329/335 (98%)	-1.09	0	100 100	27, 43, 67, 87	0
1	C	327/335 (97%)	-0.07	20 (6%)	28 26	30, 63, 134, 172	0
1	D	329/335 (98%)	-0.03	21 (6%)	27 24	30, 63, 162, 188	0
All	All	1314/1340 (98%)	-0.57	41 (3%)	51 49	27, 49, 130, 188	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	PHE	3.9
1	D	268	ALA	3.9
1	D	242	VAL	3.7
1	D	236	ALA	3.4
1	D	272	VAL	3.3
1	D	280	PHE	3.3
1	C	242	VAL	3.1
1	D	246	HIS	3.0
1	D	232	ALA	2.9
1	C	285	THR	2.9
1	D	256	ILE	2.8
1	D	277	LEU	2.8
1	D	181	ASN	2.8
1	C	236	ALA	2.8
1	D	248	ILE	2.7
1	D	260	LEU	2.7
1	D	228	VAL	2.6
1	C	269	PHE	2.5
1	D	279	ALA	2.5
1	D	233	PHE	2.5
1	C	276	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	235	ALA	2.4
1	D	250	MET	2.4
1	C	279	ALA	2.4
1	C	228	VAL	2.4
1	C	289	VAL	2.4
1	D	243	LEU	2.3
1	C	187	ALA	2.3
1	D	290	VAL	2.3
1	C	256	ILE	2.3
1	D	257	ARG	2.3
1	C	277	LEU	2.3
1	C	248	ILE	2.2
1	C	185	PHE	2.2
1	C	261	LYS	2.1
1	C	232	ALA	2.1
1	C	262	SER	2.1
1	C	243	LEU	2.1
1	D	255	ALA	2.1
1	C	255	ALA	2.0
1	D	185	PHE	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 oligosaccharides 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.