



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:49 AM UTC

PDB ID : 3CAW / pdb_00003caw
Title : Crystal structure of o-succinylbenzoate synthase from *Bdellovibrio bacteriovorus* liganded with Mg
Authors : Fedorov, A.A.; Fedorov, E.V.; Sakai, A.; Burley, S.K.; Gerlt, J.A.; Almo, S.C.;
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Deposited on : 2008-02-20
Resolution : 1.87 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	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

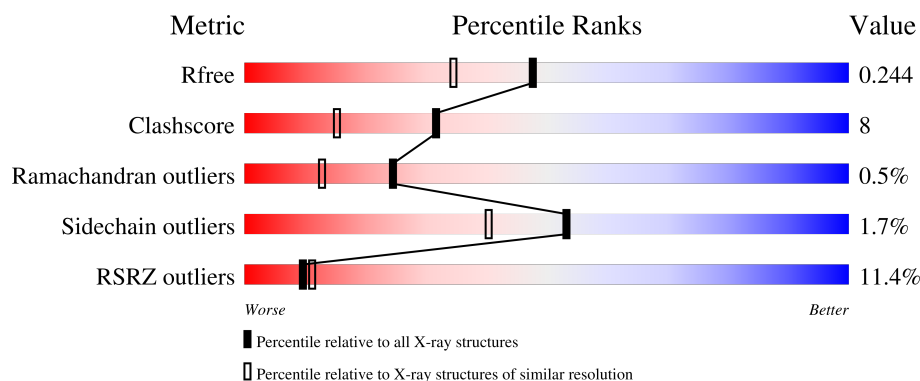
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	330	8% 79% 16% • •
1	B	330	13% 76% 18% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5314 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 o-succinylbenzoate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2535	1637	427	458	13			
1	B	316	Total	C	N	O	S	0	0	0
			2535	1637	427	458	13			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

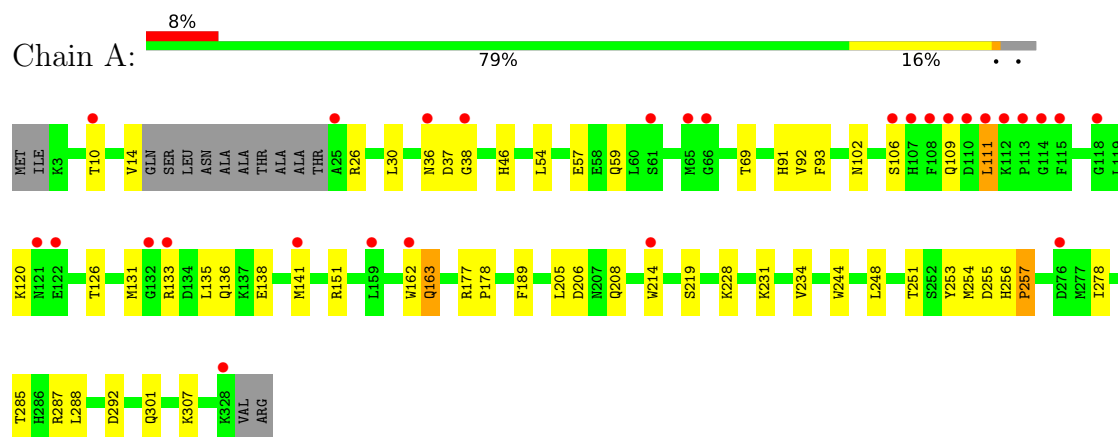
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total	O	0	0
			118	118		
3	B	124	Total	O	0	0
			124	124		

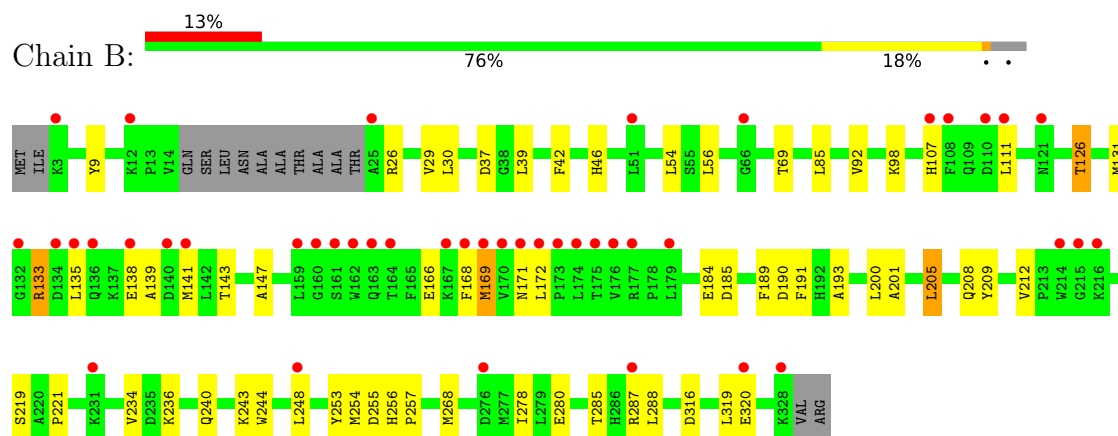
3 Residue-property plots

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: o-succinylbenzoate synthase



• Molecule 1: o-succinylbenzoate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.38Å 78.61Å 78.46Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	24.85 – 1.87 24.85 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.1 (24.85-1.87) 97.3 (24.85-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.61 (at 1.87Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.244 0.219 , 0.244	Depositor DCC
R_{free} test set	2645 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,-l,-k 0.010 for -h,l,k 0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5314	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: MG

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	0.34	0/2596	0.83	5/3507 (0.1%)
1	B	0.33	0/2596	0.84	6/3507 (0.2%)
All	All	0.34	0/5192	0.84	11/7014 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	THR	N-CA-C	-6.42	102.05	110.53
1	B	169	MET	N-CA-C	6.39	118.78	111.11
1	B	54	LEU	N-CA-C	-6.33	101.57	110.50
1	B	234	VAL	N-CA-C	5.85	116.32	110.23
1	A	30	LEU	N-CA-C	-5.78	101.14	110.32
1	B	212	VAL	N-CA-C	5.74	113.56	107.76
1	A	54	LEU	N-CA-C	-5.62	102.17	110.48
1	A	234	VAL	N-CA-C	5.29	115.50	110.42
1	A	214	TRP	N-CA-C	5.27	118.50	111.75
1	B	30	LEU	N-CA-C	-5.18	102.08	110.32
1	A	292	ASP	N-CA-C	-5.05	102.41	109.69

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	2535	0	2545	41	0
1	B	2535	0	2545	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	118	0	0	2	0
3	B	124	0	0	0	0
All	All	5314	0	5090	82	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 8.

All (82) 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:26:ARG:HE	1:A:46:HIS:HE1	1.17	0.90
1:B:26:ARG:HE	1:B:46:HIS:HE1	1.14	0.86
1:A:14:VAL:HG13	1:B:147:ALA:HA	1.61	0.82
1:A:163:GLN:NE2	1:A:163:GLN:H	1.80	0.79
1:A:163:GLN:H	1:A:163:GLN:HE21	1.30	0.77
1:A:248:LEU:HD11	1:A:278:ILE:HD12	1.65	0.76
1:B:248:LEU:HD11	1:B:278:ILE:HD12	1.67	0.76
1:B:169:MET:HA	1:B:172:LEU:HD23	1.69	0.75
1:A:177:ARG:HB2	1:A:178:PRO:HD3	1.73	0.71
1:B:107:HIS:CE1	1:B:138:GLU:HG2	2.26	0.71
1:A:189:PHE:H	1:A:208:GLN:HE21	1.41	0.68
1:B:189:PHE:H	1:B:208:GLN:HE21	1.40	0.67
1:A:189:PHE:H	1:A:208:GLN:NE2	1.95	0.64
1:A:26:ARG:HE	1:A:46:HIS:CE1	2.08	0.63
1:B:219:SER:HA	1:B:244:TRP:CZ3	2.35	0.61
1:A:111:LEU:HD22	1:A:141:MET:SD	2.45	0.56
1:A:228:LYS:HG2	1:A:251:THR:OG1	2.06	0.55
1:B:133:ARG:HA	1:B:133:ARG:HE	1.71	0.55
1:B:37:ASP:CG	1:B:39:LEU:HD13	2.32	0.54
1:A:136:GLN:H	1:A:136:GLN:CD	2.16	0.53
1:A:206:ASP:OD1	1:A:228:LYS:HE3	2.08	0.53
1:A:219:SER:HA	1:A:244:TRP:CZ3	2.44	0.53
1:A:36:ASN:C	1:A:38:GLY:H	2.16	0.53
1:B:236:LYS:O	1:B:240:GLN:HG3	2.10	0.52
1:B:26:ARG:HE	1:B:46:HIS:CE1	2.07	0.52
1:B:190:ASP:HB3	1:B:193:ALA:HB3	1.91	0.52
1:A:126:THR:HG21	3:A:437:HOH:O	2.10	0.52
1:A:57:GLU:H	1:A:57:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:HE2	1:B:201:ALA:HB2	1.93	0.51
1:A:285:THR:HB	1:A:288:LEU:HD12	1.93	0.51
1:B:107:HIS:NE2	1:B:138:GLU:HG2	2.26	0.51
1:B:111:LEU:HD11	1:B:141:MET:HE2	1.92	0.50
1:B:42:PHE:CD2	1:B:319:LEU:HD13	2.47	0.49
1:A:126:THR:HG22	1:A:151:ARG:HB2	1.94	0.49
1:B:135:LEU:HD22	1:B:168:PHE:CD1	2.47	0.49
1:B:184:GLU:O	1:B:185:ASP:C	2.56	0.49
1:B:255:ASP:OD1	1:B:255:ASP:N	2.41	0.49
1:A:287:ARG:HH11	1:A:287:ARG:HG2	1.78	0.48
1:B:316:ASP:O	1:B:320:GLU:HG3	2.13	0.48
1:A:26:ARG:NE	1:A:46:HIS:HE1	1.98	0.48
1:B:189:PHE:H	1:B:208:GLN:NE2	2.09	0.48
1:B:205:LEU:HD11	1:B:209:TYR:HA	1.94	0.48
1:A:135:LEU:HD12	1:A:135:LEU:N	2.29	0.48
1:A:248:LEU:C	1:A:248:LEU:HD12	2.39	0.47
1:A:102:ASN:HB3	1:A:126:THR:OG1	2.14	0.47
1:A:36:ASN:O	1:A:38:GLY:N	2.47	0.47
1:A:131:MET:HA	1:A:138:GLU:OE1	2.15	0.47
1:B:139:ALA:O	1:B:143:THR:HG23	2.15	0.47
1:B:29:VAL:HG13	1:B:56:LEU:HD21	1.97	0.46
1:B:171:ASN:HD22	1:B:171:ASN:N	2.12	0.46
1:B:126:THR:HG23	1:B:280:GLU:OE1	2.15	0.46
1:B:98:LYS:HA	1:B:268:MET:HE2	1.98	0.46
1:A:69:THR:HG23	3:A:505:HOH:O	2.14	0.46
1:A:248:LEU:CD1	1:A:278:ILE:HD12	2.43	0.45
1:B:285:THR:HB	1:B:288:LEU:HD12	1.97	0.45
1:B:131:MET:HA	1:B:138:GLU:OE1	2.17	0.45
1:A:255:ASP:OD1	1:A:255:ASP:N	2.44	0.44
1:A:136:GLN:CD	1:A:136:GLN:N	2.75	0.44
1:B:191:PHE:CE1	1:B:221:PRO:HD3	2.52	0.44
1:A:92:VAL:HG13	1:A:93:PHE:HD1	1.82	0.44
1:B:9:TYR:CD2	1:B:9:TYR:C	2.96	0.44
1:B:248:LEU:C	1:B:248:LEU:HD12	2.42	0.44
1:A:91:HIS:HB3	1:A:307:LYS:HE3	2.00	0.43
1:B:243:LYS:HE2	1:B:244:TRP:CZ2	2.53	0.43
1:B:248:LEU:CD1	1:B:278:ILE:HD12	2.44	0.43
1:A:231:LYS:HE2	1:A:231:LYS:HB3	1.82	0.43
1:B:256:HIS:CG	1:B:257:PRO:HD2	2.52	0.43
1:B:168:PHE:O	1:B:172:LEU:HD22	2.19	0.42
1:A:10:THR:HA	1:A:26:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:TYR:O	1:B:254:MET:C	2.62	0.42
1:A:163:GLN:HE21	1:A:163:GLN:N	2.07	0.42
1:A:256:HIS:CG	1:A:257:PRO:HD2	2.55	0.42
1:A:287:ARG:HG2	1:A:287:ARG:NH1	2.35	0.42
1:A:59:GLN:HG2	1:A:69:THR:HG21	2.01	0.42
1:A:106:SER:HB3	1:A:109:GLN:HE21	1.85	0.41
1:B:287:ARG:HH11	1:B:287:ARG:HG2	1.86	0.41
1:A:36:ASN:C	1:A:38:GLY:N	2.77	0.41
1:B:85:LEU:HD13	1:B:92:VAL:HA	2.02	0.41
1:B:39:LEU:HD12	1:B:39:LEU:N	2.36	0.40
1:B:166:GLU:HG3	1:B:200:LEU:HD11	2.02	0.40
1:B:171:ASN:N	1:B:171:ASN:ND2	2.68	0.40
1:A:253:TYR:O	1:A:254:MET:C	2.65	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	312/330 (94%)	297 (95%)	12 (4%)	3 (1%)	12	3
1	B	312/330 (94%)	293 (94%)	19 (6%)	0	100	100
All	All	624/660 (94%)	590 (95%)	31 (5%)	3 (0%)	24	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	111	LEU
1	A	133	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	270/280 (96%)	264 (98%)	6 (2%)	45	30
1	B	270/280 (96%)	267 (99%)	3 (1%)	65	56
All	All	540/560 (96%)	531 (98%)	9 (2%)	53	40

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

Mol	Chain	Res	Type
1	A	120	LYS
1	A	162	TRP
1	A	163	GLN
1	A	205	LEU
1	A	257	PRO
1	A	301	GLN
1	B	126	THR
1	B	133	ARG
1	B	205	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	107	HIS
1	A	109	GLN
1	A	121	ASN
1	A	157	ASN
1	A	163	GLN
1	A	208	GLN
1	B	46	HIS
1	B	171	ASN
1	B	208	GLN
1	B	242	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [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	316/330 (95%)	0.57	28 (8%) 15 17	11, 21, 46, 60	0
1	B	316/330 (95%)	0.65	44 (13%) 6 6	11, 22, 46, 58	0
All	All	632/660 (95%)	0.61	72 (11%) 10 11	11, 21, 46, 60	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ASN	6.4
1	A	162	TRP	5.4
1	A	108	PHE	5.4
1	B	162	TRP	5.3
1	A	107	HIS	5.3
1	B	172	LEU	5.1
1	B	108	PHE	5.0
1	A	115	PHE	4.8
1	B	170	VAL	4.8
1	A	114	GLY	4.7
1	B	328	LYS	4.5
1	B	174	LEU	4.5
1	A	109	GLN	4.2
1	A	328	LYS	4.2
1	B	173	PRO	4.1
1	B	134	ASP	4.0
1	B	171	ASN	3.9
1	B	175	THR	3.9
1	B	167	LYS	3.7
1	B	159	LEU	3.7
1	B	107	HIS	3.7
1	B	214	TRP	3.7
1	B	161	SER	3.6
1	A	106	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	112	LYS	3.5
1	B	164	THR	3.4
1	B	160	GLY	3.4
1	B	141	MET	3.4
1	A	113	PRO	3.4
1	B	176	VAL	3.3
1	A	122	GLU	3.3
1	B	140	ASP	3.3
1	A	65	MET	3.3
1	B	111	LEU	3.3
1	A	110	ASP	3.2
1	A	38	GLY	3.1
1	A	121	ASN	3.0
1	B	169	MET	3.0
1	B	132	GLY	2.9
1	A	159	LEU	2.9
1	B	216	LYS	2.9
1	A	111	LEU	2.8
1	A	25	ALA	2.8
1	A	118	GLY	2.8
1	B	25	ALA	2.7
1	A	214	TRP	2.7
1	A	132	GLY	2.7
1	A	141	MET	2.5
1	B	168	PHE	2.5
1	B	136	GLN	2.5
1	B	138	GLU	2.5
1	B	163	GLN	2.5
1	B	215	GLY	2.4
1	A	133	ARG	2.4
1	B	66	GLY	2.4
1	B	110	ASP	2.3
1	A	276	ASP	2.2
1	B	177	ARG	2.2
1	B	320	GLU	2.2
1	A	61	SER	2.2
1	B	287	ARG	2.2
1	B	248	LEU	2.1
1	B	12	LYS	2.1
1	B	3	LYS	2.1
1	B	231	LYS	2.1
1	B	121	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	2.1
1	B	135	LEU	2.0
1	B	179	LEU	2.0
1	B	276	ASP	2.0
1	A	10	THR	2.0
1	A	66	GLY	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](#)

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($\text{\AA}^2$)	Q<0.9
2	MG	B	401	1/1	0.94	0.14	29,29,29,29	0
2	MG	A	401	1/1	0.95	0.12	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.