



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:39 AM GMT

PDB ID : 3FK4
Title : Crystal structure of RuBisCO-like protein from Bacillus Cereus ATCC 14579
Authors : Fedorov, A.A.; Fedorov, E.V.; Imker, H.J.; Burley, S.K.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-12-15
Resolution : 2.00 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

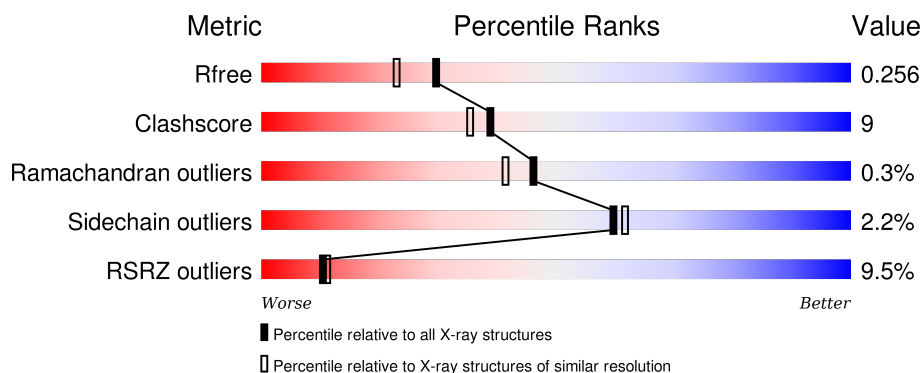
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	414	<div> <div>5%</div> <div>78%</div> <div>15%</div> <div>6%</div> </div>
1	B	414	<div> <div>13%</div> <div>73%</div> <div>20%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6206 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 RuBisCO-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3009	1937	511	558	3			
1	B	391	Total	C	N	O	S	0	0	0
			3037	1959	516	559	3			

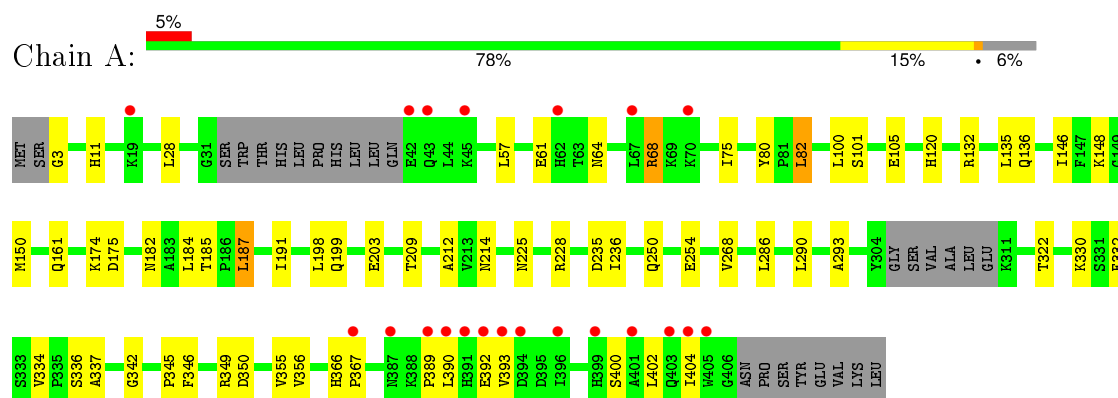
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		
2	B	49	Total	O	0	0
			49	49		

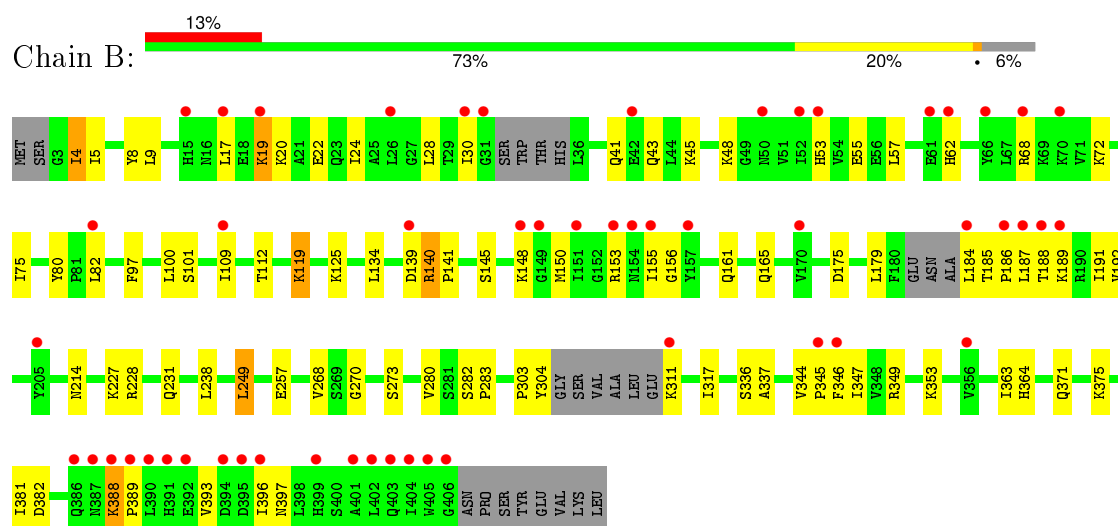
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: RuBisCO-like protein



• Molecule 1: RuBisCO-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.92Å 115.67Å 116.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.67 – 2.00 29.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.67-2.00) 99.5 (29.66-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.257 0.235 , 0.256	Depositor DCC
R_{free} test set	3560 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 70779 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6206	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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	0.35	0/3072	0.61	0/4154
1	B	0.31	0/3101	0.58	0/4193
All	All	0.33	0/6173	0.59	0/8347

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	3009	0	3048	47	0
1	B	3037	0	3085	64	0
2	A	111	0	0	3	0
2	B	49	0	0	1	0
All	All	6206	0	6133	109	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 9.

All (109) 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:B:9:LEU:HB2	1:B:109:ILE:HD11	1.29	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LYS:H	1:B:161:GLN:HE22	1.04	0.93
1:A:148:LYS:H	1:A:161:GLN:HE22	1.31	0.78
1:A:349:ARG:HG3	1:A:350:ASP:N	1.99	0.78
1:B:19:LYS:HA	1:B:19:LYS:HE3	1.66	0.75
1:B:283:PRO:HA	1:B:317:ILE:HG12	1.72	0.72
1:B:381:ILE:HD12	1:B:382:ASP:N	2.07	0.70
1:B:303:PRO:HB2	1:B:311:LYS:HG2	1.75	0.69
1:A:182:ASN:HD21	1:A:185:THR:H	1.42	0.67
1:A:61:GLU:HA	1:A:64:ASN:HD22	1.61	0.66
1:B:184:LEU:HD23	1:B:184:LEU:O	1.96	0.65
1:B:148:LYS:H	1:B:161:GLN:NE2	1.88	0.64
1:A:182:ASN:ND2	1:A:185:THR:H	1.97	0.63
1:A:28:LEU:HD11	1:A:100:LEU:HD13	1.80	0.62
1:B:57:LEU:HD11	1:B:75:ILE:HG12	1.82	0.61
1:B:140:ARG:HG3	1:B:381:ILE:HD13	1.84	0.59
1:B:150:MET:HE3	1:B:153:ARG:HB2	1.85	0.58
1:A:198:LEU:HD22	1:A:209:THR:HB	1.85	0.58
1:A:57:LEU:HD11	1:A:75:ILE:HG13	1.86	0.57
1:A:235:ASP:O	1:A:236:ILE:HD13	2.05	0.57
1:B:388:LYS:HB2	1:B:388:LYS:NZ	2.19	0.57
1:B:282:SER:N	1:B:283:PRO:HD2	2.20	0.57
1:B:5:ILE:HB	1:B:112:THR:OG1	2.05	0.56
1:B:140:ARG:HG2	1:B:141:PRO:O	2.07	0.55
1:B:119:LYS:NZ	1:B:119:LYS:HB2	2.22	0.54
1:A:187:LEU:HD22	1:A:191:ILE:CD1	2.38	0.53
1:B:148:LYS:N	1:B:161:GLN:HE22	1.88	0.53
1:A:400:SER:O	1:A:404:ILE:HG13	2.09	0.52
1:A:349:ARG:HG3	1:A:350:ASP:H	1.74	0.52
1:B:139:ASP:CG	1:B:140:ARG:H	2.12	0.52
1:A:174:LYS:NZ	2:A:486:HOH:O	2.39	0.52
1:B:68:ARG:HH11	1:B:68:ARG:HG3	1.75	0.52
1:B:336:SER:O	1:B:337:ALA:HB3	2.11	0.51
1:A:389:PRO:HB2	1:A:392:GLU:HG3	1.93	0.51
1:A:28:LEU:HD11	1:A:100:LEU:CD1	2.41	0.51
1:B:4:ILE:HD13	1:B:5:ILE:N	2.26	0.51
1:B:227:LYS:HE2	1:B:257:GLU:HB2	1.92	0.51
1:A:11:HIS:HB2	1:A:105:GLU:HB3	1.93	0.51
1:A:199:GLN:HE21	1:A:203:GLU:HG3	1.76	0.51
1:B:17:LEU:HG	1:B:72:LYS:HD2	1.92	0.50
1:B:249:LEU:O	1:B:249:LEU:HD22	2.12	0.50
1:A:212:ALA:HA	1:A:236:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:HIS:HD2	2:A:477:HOH:O	1.95	0.49
1:A:182:ASN:HD22	1:A:184:LEU:H	1.60	0.49
1:A:68:ARG:HD2	1:B:62:HIS:ND1	2.28	0.49
1:B:186:PRO:O	1:B:189:LYS:HB3	2.13	0.49
1:B:303:PRO:HB3	1:B:311:LYS:HA	1.95	0.48
1:A:334:VAL:HG22	1:A:356:VAL:HB	1.96	0.48
1:B:363:ILE:HG13	1:B:364:HIS:N	2.29	0.48
1:A:346:PHE:HA	1:A:349:ARG:HG2	1.96	0.47
1:A:336:SER:O	1:A:337:ALA:HB3	2.14	0.47
1:B:53:HIS:NE2	1:B:55:GLU:HB2	2.29	0.47
1:B:30:ILE:HD12	1:B:30:ILE:O	2.14	0.47
1:A:355:VAL:HG22	1:A:356:VAL:N	2.29	0.47
1:B:30:ILE:HG13	1:B:48:LYS:HA	1.96	0.47
1:A:150:MET:HE1	1:A:175:ASP:OD1	2.15	0.47
1:B:396:ILE:HG13	1:B:397:ASN:N	2.29	0.47
1:B:214:ASN:HA	1:B:238:LEU:HB3	1.97	0.46
1:B:184:LEU:HD22	1:B:185:THR:HG23	1.98	0.46
1:B:311:LYS:HD3	1:B:311:LYS:O	2.16	0.46
1:B:43:GLN:NE2	2:B:453:HOH:O	2.48	0.46
1:B:41:GLN:O	1:B:45:LYS:HG2	2.16	0.45
1:B:344:VAL:HB	1:B:345:PRO:HD3	1.98	0.45
1:A:225:ASN:HD22	1:A:228:ARG:HH11	1.65	0.45
1:B:139:ASP:CG	1:B:140:ARG:N	2.70	0.45
1:B:228:ARG:NH1	1:B:231:GLN:HE22	2.15	0.45
1:A:342:GLY:O	1:A:345:PRO:HD2	2.16	0.45
1:A:250:GLN:O	1:A:254:GLU:HG3	2.17	0.45
1:B:304:TYR:CE2	1:B:347:ILE:HG12	2.52	0.45
1:B:186:PRO:O	1:B:189:LYS:N	2.50	0.44
1:B:304:TYR:HE2	1:B:347:ILE:HG12	1.83	0.44
1:B:20:LYS:O	1:B:24:ILE:HG13	2.17	0.44
1:A:28:LEU:HD12	1:A:80:TYR:OH	2.18	0.44
1:B:28:LEU:HD12	1:B:80:TYR:OH	2.17	0.44
1:A:367:PRO:HD3	1:A:404:ILE:HD12	1.99	0.44
1:B:145:SER:OG	1:B:165:GLN:NE2	2.51	0.44
1:A:366:HIS:CG	1:A:367:PRO:HD2	2.53	0.44
1:A:290:LEU:HD11	2:A:498:HOH:O	2.18	0.44
1:B:45:LYS:O	1:B:48:LYS:HG2	2.17	0.44
1:A:390:LEU:HB3	1:A:402:LEU:HD11	1.99	0.43
1:B:155:ILE:HG23	1:B:156:GLY:N	2.33	0.43
1:B:8:TYR:CE1	1:B:100:LEU:HD23	2.54	0.43
1:B:82:LEU:HD23	1:B:82:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASP:HB3	1:B:179:LEU:HD11	2.00	0.43
1:A:132:ARG:O	1:A:136:GLN:N	2.52	0.42
1:A:225:ASN:ND2	1:A:228:ARG:HH11	2.17	0.42
1:B:165:GLN:HG2	1:B:363:ILE:CD1	2.50	0.42
1:B:388:LYS:HE3	1:B:393:VAL:HG22	2.01	0.42
1:B:97:PHE:O	1:B:101:SER:HB3	2.19	0.42
1:A:146:ILE:HG12	1:A:174:LYS:HG2	2.02	0.42
1:A:389:PRO:O	1:A:393:VAL:HG23	2.20	0.42
1:B:371:GLN:O	1:B:375:LYS:HG3	2.20	0.42
1:B:22:GLU:OE1	1:B:22:GLU:HA	2.20	0.42
1:B:228:ARG:NH1	1:B:231:GLN:NE2	2.68	0.41
1:B:388:LYS:HA	1:B:389:PRO:HD3	1.95	0.41
1:B:187:LEU:O	1:B:191:ILE:HG13	2.20	0.41
1:A:187:LEU:HD22	1:A:191:ILE:HD11	2.01	0.41
1:A:286:LEU:HA	1:A:290:LEU:HD12	2.02	0.41
1:A:322:THR:O	1:A:330:LYS:HE2	2.20	0.41
1:B:150:MET:CE	1:B:153:ARG:HB2	2.50	0.41
1:B:188:THR:O	1:B:192:VAL:HG23	2.20	0.41
1:B:273:SER:HB3	1:B:280:VAL:O	2.21	0.41
1:A:346:PHE:O	1:A:349:ARG:HG2	2.21	0.41
1:A:250:GLN:HA	1:A:293:ALA:O	2.21	0.41
1:A:290:LEU:HA	1:A:290:LEU:HD23	1.95	0.40
1:A:101:SER:O	1:B:270:GLY:HA3	2.21	0.40
1:A:3:GLY:HA2	1:A:82:LEU:HD23	2.02	0.40
1:A:135:LEU:O	1:A:136:GLN:HB2	2.22	0.40
1:B:346:PHE:O	1:B:349:ARG: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	382/414 (92%)	366 (96%)	15 (4%)	1 (0%)	46	41
1	B	383/414 (92%)	367 (96%)	15 (4%)	1 (0%)	46	41
All	All	765/828 (92%)	733 (96%)	30 (4%)	2 (0%)	46	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	B	268	VAL

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	322/346 (93%)	317 (98%)	5 (2%)	70	73
1	B	326/346 (94%)	317 (97%)	9 (3%)	51	50
All	All	648/692 (94%)	634 (98%)	14 (2%)	60	62

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	82	LEU
1	A	187	LEU
1	A	214	ASN
1	A	332	PHE
1	B	4	ILE
1	B	19	LYS
1	B	119	LYS
1	B	125	LYS
1	B	134	LEU
1	B	140	ARG
1	B	249	LEU
1	B	353	LYS
1	B	388	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	47	HIS
1	A	50	ASN
1	A	60	HIS
1	A	62	HIS
1	A	120	HIS
1	A	133	ASN
1	A	161	GLN
1	A	182	ASN
1	A	199	GLN
1	A	214	ASN
1	A	225	ASN
1	A	397	ASN
1	B	23	GLN
1	B	41	GLN
1	B	50	ASN
1	B	133	ASN
1	B	138	HIS
1	B	161	GLN
1	B	165	GLN
1	B	231	GLN
1	B	386	GLN
1	B	397	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	388/414 (93%)	0.30	21 (5%) 29 31	23, 37, 68, 77	0
1	B	391/414 (94%)	0.72	53 (13%) 4 4	26, 49, 71, 80	0
All	All	779/828 (94%)	0.51	74 (9%) 10 11	23, 44, 70, 80	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	LEU	5.9
1	B	31	GLY	5.7
1	B	391	HIS	4.8
1	B	151	ILE	4.7
1	A	42	GLU	4.5
1	B	405	TRP	4.5
1	B	403	GLN	4.4
1	B	26	LEU	4.2
1	A	391	HIS	3.9
1	B	30	ILE	3.9
1	B	62	HIS	3.8
1	A	45	LYS	3.7
1	B	399	HIS	3.6
1	B	346	PHE	3.5
1	B	396	ILE	3.5
1	A	43	GLN	3.4
1	B	404	ILE	3.4
1	B	155	ILE	3.2
1	A	403	GLN	3.2
1	A	399	HIS	3.1
1	B	68	ARG	3.0
1	B	406	GLY	2.9
1	A	396	ILE	2.9
1	A	19	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	70	LYS	2.9
1	A	392	GLU	2.9
1	B	356	VAL	2.9
1	B	153	ARG	2.9
1	B	148	LYS	2.8
1	B	187	LEU	2.7
1	B	388	LYS	2.7
1	B	139	ASP	2.7
1	B	188	THR	2.7
1	B	53	HIS	2.6
1	A	394	ASP	2.6
1	A	367	PRO	2.6
1	B	154	ASN	2.6
1	B	392	GLU	2.5
1	A	387	ASN	2.5
1	A	62	HIS	2.5
1	B	42	GLU	2.5
1	A	393	VAL	2.5
1	A	404	ILE	2.5
1	B	189	LYS	2.5
1	A	70	LYS	2.4
1	B	390	LEU	2.4
1	B	149	GLY	2.3
1	A	405	TRP	2.3
1	B	389	PRO	2.3
1	B	394	ASP	2.3
1	B	15	HIS	2.3
1	B	401	ALA	2.2
1	B	19	LYS	2.2
1	A	401	ALA	2.2
1	A	67	LEU	2.2
1	B	82	LEU	2.2
1	B	395	ASP	2.2
1	B	50	ASN	2.2
1	A	389	PRO	2.1
1	B	402	LEU	2.1
1	B	345	PRO	2.1
1	B	52	ILE	2.1
1	B	17	LEU	2.1
1	B	311	LYS	2.1
1	B	186	PRO	2.1
1	B	66	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	390	LEU	2.1
1	B	157	TYR	2.1
1	B	205	TYR	2.1
1	B	61	GLU	2.0
1	B	387	ASN	2.0
1	B	386	GLN	2.0
1	B	170	VAL	2.0
1	B	109	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.