W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:09 PM GMT

PDB ID : 1IZ1
Title : CRYSTAL STRUCTURE OF CBNR, A LYSR FAMILY TRANSCRIP-
TIONAL REGULATOR
Authors : Muraoka, S.; Okumura, R.; Ogawa, N.; Miyashita, K.; Senda, T.
Deposited on : 2002-09-18
Resolution : 2.50 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		4
Ramachandran outliers		0.7%
Sidechain outliers		9.0%
RSRZ outliers		4.8%

Worse · *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
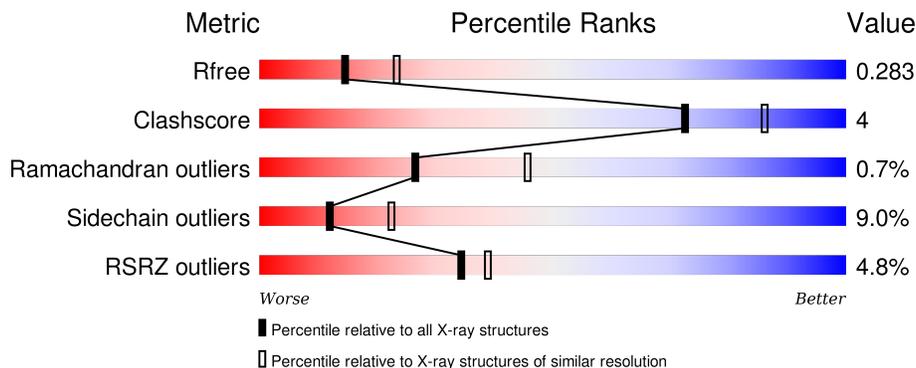
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	294	84% 14% •••
1	B	294	3% 82% 17% •
1	P	294	3% 84% 13% ••
1	Q	294	13% 78% 18% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9097 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 LysR-type regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total 2241	C 1425	N 415	O 394	S 7	0	0	0
1	B	294	Total 2259	C 1435	N 418	O 399	S 7	0	0	0
1	P	292	Total 2241	C 1425	N 415	O 394	S 7	0	0	0
1	Q	292	Total 2241	C 1425	N 415	O 394	S 7	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total 34	O 34	0	0
2	B	30	Total 30	O 30	0	0
2	P	27	Total 27	O 27	0	0
2	Q	24	Total 24	O 24	0	0

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: LysR-type regulatory protein
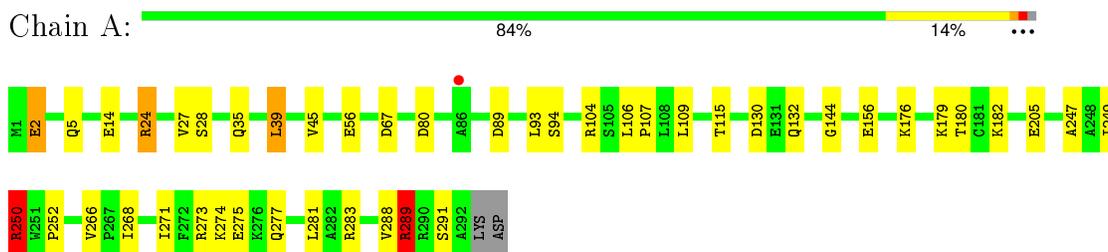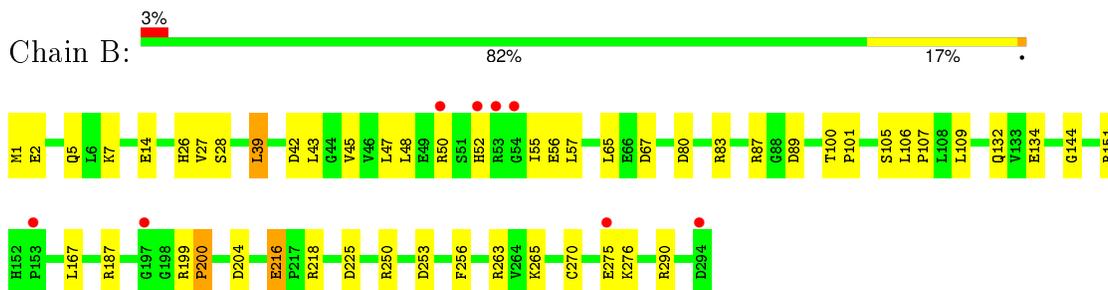
- Molecule 1: LysR-type regulatory protein

- Molecule 1: LysR-type regulatory protein

- Molecule 1: LysR-type regulatory protein

R70 L74 D80 R87 G88 D89 V90 A96 G99 T100 P101 L106 P107 R111 L124 T125 T128 Q132 H142 V143 G144 F145 S146 R147 F148 F149 N159 Q162 L165 L209 R221 R250 W251 P252 D253 G261 T262 R263 V264 K265 V266 P267

I268 I271 E275 L281 R289 R290 S291 A292 LYS ASP
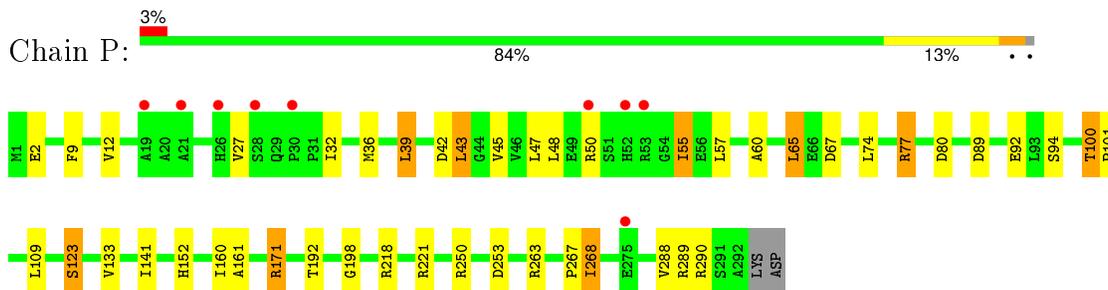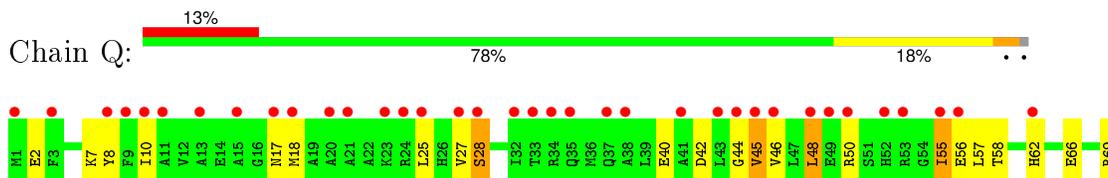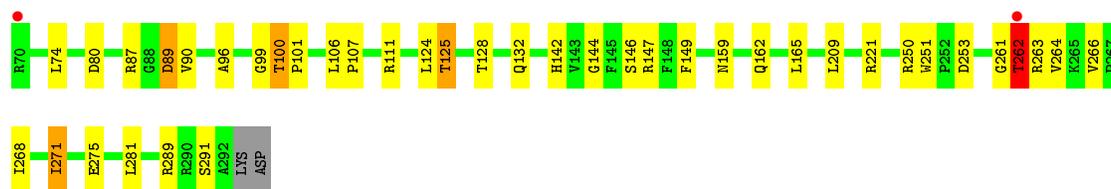
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.27Å 124.48Å 166.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 43.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.50) 97.8 (43.49-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.222 , 0.286 0.224 , 0.283	Depositor DCC
R_{free} test set	2374 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 46796 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9097	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.65	0/2285	0.87	5/3092 (0.2%)
1	B	0.64	1/2303 (0.0%)	0.81	6/3114 (0.2%)
1	P	0.65	0/2285	0.82	7/3092 (0.2%)
1	Q	0.63	0/2285	0.82	4/3092 (0.1%)
All	All	0.64	1/9158 (0.0%)	0.83	22/12390 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
1	Q	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	GLU	CD-OE2	5.70	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	80	ASP	CB-CG-OD2	7.13	124.71	118.30
1	A	67	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	67	ASP	CB-CG-OD2	6.73	124.35	118.30
1	B	80	ASP	CB-CG-OD2	6.72	124.35	118.30
1	Q	89	ASP	CB-CG-OD2	6.61	124.25	118.30
1	Q	80	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	204	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	89	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	80	ASP	CB-CG-OD2	6.22	123.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	89	ASP	CB-CG-OD2	6.00	123.70	118.30
1	P	77	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	Q	253	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	130	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	42	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	225	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	250	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	P	77	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	P	67	ASP	CB-CG-OD2	5.17	122.96	118.30
1	P	65	LEU	CA-CB-CG	5.12	127.09	115.30
1	P	42	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	253	ASP	CB-CG-OD2	5.09	122.89	118.30
1	Q	42	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	198	GLY	Peptide
1	Q	261	GLY	Peptide

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	2241	0	2313	15	0
1	B	2259	0	2330	14	0
1	P	2241	0	2313	21	0
1	Q	2241	0	2313	27	0
2	A	34	0	0	0	0
2	B	30	0	0	2	0
2	P	27	0	0	0	0
2	Q	24	0	0	0	0
All	All	9097	0	9269	76	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 4.

All (76) 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:Q:262:THR:O	1:Q:264:VAL:HG23	1.70	0.90
1:Q:149:PHE:CE1	1:Q:271:ILE:HD13	2.23	0.73
1:Q:159:ASN:HD21	1:Q:162:GLN:HE21	1.39	0.71
1:A:247:ALA:O	1:A:250:ARG:NH2	2.27	0.68
1:B:83:ARG:NH1	2:B:301:HOH:O	2.28	0.66
1:A:132:GLN:NE2	1:A:144:GLY:HA3	2.11	0.65
1:P:39:LEU:HD22	1:P:43:LEU:HD22	1.79	0.64
1:Q:165:LEU:HD21	1:Q:266:VAL:HG21	1.82	0.62
1:Q:100:THR:N	1:Q:101:PRO:CD	2.65	0.59
1:B:187:ARG:O	1:B:218:ARG:HD2	2.04	0.58
1:Q:149:PHE:CZ	1:Q:271:ILE:HD13	2.40	0.57
1:A:5:GLN:HB3	1:A:39:LEU:HG	1.85	0.57
1:Q:132:GLN:NE2	1:Q:144:GLY:HA3	2.19	0.57
1:B:27:VAL:HG12	1:B:28:SER:O	2.05	0.56
1:Q:99:GLY:C	1:Q:101:PRO:HD2	2.26	0.56
1:A:14:GLU:OE2	1:A:24:ARG:NH2	2.40	0.55
1:Q:57:LEU:HB2	1:Q:62:HIS:CE1	2.41	0.55
1:A:250:ARG:NH1	1:A:250:ARG:HA	2.22	0.55
1:A:2:GLU:HG3	2:B:306:HOH:O	2.07	0.54
1:P:133:VAL:HG11	1:P:152:HIS:CD2	2.42	0.54
1:P:161:ALA:HB3	1:P:268:ILE:CD1	2.38	0.54
1:P:45:VAL:HG11	1:P:60:ALA:HB1	1.90	0.52
1:P:109:LEU:HD21	1:P:288:VAL:HG12	1.90	0.52
1:Q:159:ASN:HD21	1:Q:162:GLN:NE2	2.05	0.51
1:P:100:THR:N	1:P:101:PRO:CD	2.74	0.51
1:B:132:GLN:NE2	1:B:144:GLY:HA3	2.26	0.50
1:Q:209:LEU:HD11	1:Q:264:VAL:HG22	1.94	0.50
1:P:48:LEU:HD23	1:P:57:LEU:HD23	1.93	0.50
1:Q:27:VAL:O	1:Q:28:SER:CB	2.59	0.49
1:B:87:ARG:NH1	1:B:89:ASP:OD2	2.45	0.49
1:P:39:LEU:HD13	1:P:47:LEU:CD1	2.43	0.49
1:P:9:PHE:HA	1:P:36:MET:HE1	1.93	0.49
1:P:45:VAL:HG11	1:P:60:ALA:CB	2.44	0.48
1:B:167:LEU:O	1:B:256:PHE:HA	2.14	0.48
1:P:12:VAL:HG11	1:P:48:LEU:HD11	1.96	0.47
1:B:39:LEU:HD13	1:B:47:LEU:CD1	2.45	0.47
1:A:249:ILE:HD13	1:Q:251:TRP:CZ3	2.50	0.46
1:P:192:THR:HG23	1:P:221:ARG:HG3	1.96	0.46
1:Q:40:GLU:OE2	1:Q:46:VAL:HG13	2.15	0.46
1:Q:128:THR:O	1:Q:132:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:THR:N	1:B:101:PRO:CD	2.78	0.46
1:Q:142:HIS:HB3	1:Q:281:LEU:HD13	1.97	0.46
1:Q:10:ILE:HD12	1:Q:69:ARG:HG3	1.98	0.45
1:B:144:GLY:O	1:B:270:CYS:HA	2.17	0.45
1:B:1:MET:HA	1:B:5:GLN:HE22	1.82	0.45
1:Q:159:ASN:ND2	1:Q:162:GLN:HE21	2.10	0.45
1:P:48:LEU:CD2	1:P:57:LEU:HD23	2.47	0.45
1:Q:44:GLY:O	1:Q:45:VAL:HG13	2.17	0.45
1:P:161:ALA:O	1:P:267:PRO:HA	2.16	0.44
1:A:277:GLN:HG2	1:A:281:LEU:HD23	1.99	0.44
1:Q:147:ARG:NH2	1:Q:268:ILE:HD11	2.32	0.44
1:B:199:ARG:HA	1:B:200:PRO:C	2.37	0.44
1:Q:106:LEU:HB3	1:Q:107:PRO:HD3	1.99	0.44
1:P:32:ILE:O	1:P:36:MET:HG2	2.18	0.44
1:B:2:GLU:H	1:B:5:GLN:HE21	1.66	0.44
1:P:171:ARG:HG2	1:P:253:ASP:HA	2.01	0.43
1:B:106:LEU:HB3	1:B:107:PRO:HD3	1.99	0.43
1:P:77:ARG:NH1	1:P:92:GLU:OE2	2.51	0.43
1:Q:48:LEU:HA	1:Q:56:GLU:O	2.18	0.43
1:Q:27:VAL:O	1:Q:28:SER:HB2	2.20	0.42
1:A:288:VAL:O	1:A:289:ARG:C	2.58	0.42
1:P:160:ILE:HD12	1:P:160:ILE:N	2.35	0.42
1:Q:96:ALA:HA	1:Q:125:THR:O	2.20	0.42
1:P:77:ARG:HH12	1:P:123:SER:HB2	1.84	0.42
1:Q:50:ARG:HA	1:Q:55:ILE:HG22	2.00	0.41
1:P:94:SER:OG	1:P:141:ILE:HG22	2.20	0.41
1:A:106:LEU:HB3	1:A:107:PRO:HD3	2.03	0.41
1:A:250:ARG:HA	1:A:250:ARG:CZ	2.50	0.41
1:Q:8:TYR:CD1	1:Q:25:LEU:HD13	2.56	0.41
1:A:156:GLU:O	1:A:271:ILE:HA	2.21	0.41
1:A:205:GLU:HG2	1:A:266:VAL:HG12	2.02	0.41
1:B:43:LEU:HD12	1:B:47:LEU:HD11	2.03	0.40
1:Q:87:ARG:NH1	1:Q:89:ASP:OD1	2.54	0.40
1:A:5:GLN:HG2	1:A:35:GLN:HG3	2.03	0.40
1:P:48:LEU:HD13	1:P:55:ILE:HD11	2.02	0.40
1:A:179:LYS:HG3	1:A:180:THR:HG23	2.03	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	290/294 (99%)	278 (96%)	10 (3%)	2 (1%)	26	46
1	B	292/294 (99%)	275 (94%)	16 (6%)	1 (0%)	46	68
1	P	290/294 (99%)	273 (94%)	15 (5%)	2 (1%)	26	46
1	Q	290/294 (99%)	268 (92%)	19 (7%)	3 (1%)	19	34
All	All	1162/1176 (99%)	1094 (94%)	60 (5%)	8 (1%)	26	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	28	SER
1	A	104	ARG
1	A	289	ARG
1	P	55	ILE
1	Q	100	THR
1	Q	262	THR
1	P	100	THR
1	B	200	PRO

5.3.2 Protein sidechains (i)

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	229/231 (99%)	207 (90%)	22 (10%)	10	19
1	B	231/231 (100%)	208 (90%)	23 (10%)	9	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	229/231 (99%)	214 (93%)	15 (7%)	21	38
1	Q	229/231 (99%)	206 (90%)	23 (10%)	9	18
All	All	918/924 (99%)	835 (91%)	83 (9%)	12	22

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	24	ARG
1	A	27	VAL
1	A	28	SER
1	A	39	LEU
1	A	45	VAL
1	A	56	GLU
1	A	93	LEU
1	A	94	SER
1	A	109	LEU
1	A	115	THR
1	A	176	LYS
1	A	182	LYS
1	A	250	ARG
1	A	252	PRO
1	A	268	ILE
1	A	273	ARG
1	A	274	LYS
1	A	275	GLU
1	A	283	ARG
1	A	289	ARG
1	A	291	SER
1	B	7	LYS
1	B	14	GLU
1	B	26	HIS
1	B	39	LEU
1	B	45	VAL
1	B	48	LEU
1	B	50	ARG
1	B	52	HIS
1	B	55	ILE
1	B	56	GLU
1	B	57	LEU
1	B	65	LEU

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Mol	Chain	Res	Type
1	B	105	SER
1	B	109	LEU
1	B	134	GLU
1	B	151	ARG
1	B	216	GLU
1	B	250	ARG
1	B	263	ARG
1	B	265	LYS
1	B	275	GLU
1	B	276	LYS
1	B	290	ARG
1	P	2	GLU
1	P	27	VAL
1	P	39	LEU
1	P	43	LEU
1	P	50	ARG
1	P	65	LEU
1	P	74	LEU
1	P	123	SER
1	P	171	ARG
1	P	218	ARG
1	P	250	ARG
1	P	263	ARG
1	P	268	ILE
1	P	289	ARG
1	P	290	ARG
1	Q	2	GLU
1	Q	7	LYS
1	Q	17	ASN
1	Q	18	MET
1	Q	45	VAL
1	Q	48	LEU
1	Q	55	ILE
1	Q	58	THR
1	Q	66	GLU
1	Q	74	LEU
1	Q	90	VAL
1	Q	111	ARG
1	Q	124	LEU
1	Q	125	THR
1	Q	146	SER
1	Q	221	ARG

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Mol	Chain	Res	Type
1	Q	250	ARG
1	Q	262	THR
1	Q	263	ARG
1	Q	271	ILE
1	Q	275	GLU
1	Q	289	ARG
1	Q	291	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	132	GLN
1	A	159	ASN
1	A	212	HIS
1	B	5	GLN
1	B	35	GLN
1	B	37	GLN
1	B	132	GLN
1	B	212	HIS
1	P	5	GLN
1	P	126	HIS
1	P	132	GLN
1	P	277	GLN
1	Q	5	GLN
1	Q	37	GLN
1	Q	126	HIS
1	Q	132	GLN
1	Q	162	GLN
1	Q	173	GLN
1	Q	277	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 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 (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(Å²)	Q<0.9
1	A	292/294 (99%)	-0.21	1 (0%)	94 95	13, 25, 43, 52	0
1	B	294/294 (100%)	0.04	8 (2%)	58 62	14, 28, 48, 72	0
1	P	292/294 (99%)	0.10	9 (3%)	52 57	11, 29, 66, 74	0
1	Q	292/294 (99%)	0.30	38 (13%)	5 4	14, 29, 78, 83	0
All	All	1170/1176 (99%)	0.06	56 (4%)	34 39	11, 27, 67, 83	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	50	ARG	5.1
1	Q	55	ILE	4.8
1	P	52	HIS	4.4
1	B	53	ARG	4.3
1	B	54	GLY	4.2
1	B	52	HIS	4.2
1	Q	23	LYS	4.2
1	Q	25	LEU	3.9
1	Q	37	GLN	3.8
1	P	26	HIS	3.8
1	Q	13	ALA	3.8
1	Q	24	ARG	3.7
1	B	153	PRO	3.6
1	Q	17	ASN	3.5
1	Q	49	GLU	3.5
1	Q	38	ALA	3.4
1	Q	262	THR	3.3
1	Q	43	LEU	3.3
1	Q	3	PHE	3.3
1	Q	1	MET	3.3
1	Q	35	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	50	ARG	3.1
1	Q	33	THR	3.0
1	P	53	ARG	3.0
1	Q	27	VAL	2.9
1	Q	28	SER	2.9
1	P	19	ALA	2.9
1	P	275	GLU	2.8
1	Q	56	GLU	2.7
1	B	197	GLY	2.7
1	Q	44	GLY	2.7
1	Q	8	TYR	2.7
1	B	275	GLU	2.7
1	Q	20	ALA	2.7
1	Q	11	ALA	2.5
1	Q	48	LEU	2.5
1	P	21	ALA	2.5
1	Q	15	ALA	2.5
1	P	50	ARG	2.5
1	A	86	ALA	2.5
1	P	28	SER	2.5
1	Q	34	ARG	2.4
1	Q	46	VAL	2.4
1	P	30	PRO	2.4
1	Q	21	ALA	2.4
1	Q	10	ILE	2.3
1	Q	41	ALA	2.3
1	Q	45	VAL	2.2
1	Q	53	ARG	2.2
1	Q	70	ARG	2.2
1	Q	18	MET	2.2
1	Q	9	PHE	2.2
1	B	294	ASP	2.1
1	Q	32	ILE	2.1
1	Q	52	HIS	2.1
1	Q	62	HIS	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.