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

wwPDB X-ray Structure Validation Summary Report (i)

Feb 14, 2017 – 10:35 pm GMT

PDB ID	:	1ZVV
Title	:	Crystal structure of a ccpa-crh-dna complex
Authors	:	Schumacher, M.A.; Brennan, R.G.; Hillen, W.; Seidel, G.
Deposited on	:	2005-06-02
Resolution	:	2.98 Å(reported)

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

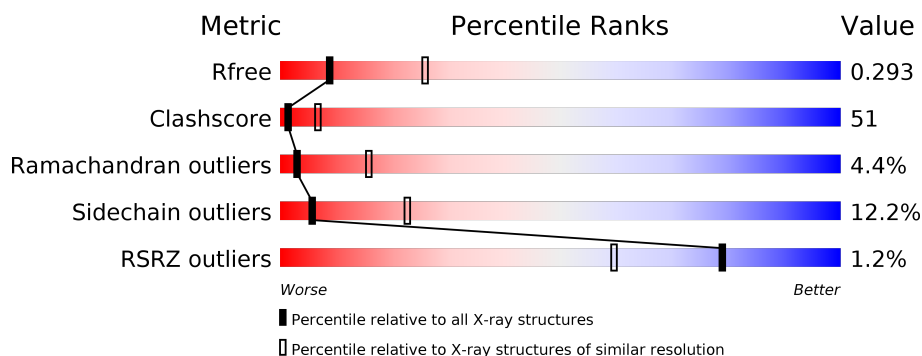|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.98 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		0.293
Clashscore		51
Ramachandran outliers		4.4%
Sidechain outliers		12.2%
RSRZ outliers		1.2%

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$_{free}$	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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	O	16	100%
1	R	16	6% / 100%
1	T	16	100%
2	A	332	% / 33% 56% 11% •
2	B	332	% / 32% 58% 10%
2	G	332	2% / 35% 54% 10% •

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Mol	Chain	Length	Quality of chain
3	J	85	35% 52% 11%
3	P	85	28% 60% 9%
3	W	85	2% 33% 53% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	G	414	-	-	-	X
4	IOD	G	418	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10661 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 DNA chain called DNA recognition strand CRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	16	Total	C	N	O	P	0	0	0
			326	156	63	92	15			
1	T	16	Total	C	N	O	P	0	0	0
			326	156	63	92	15			
1	R	16	Total	C	N	O	P	0	0	0
			326	156	63	92	15			

- Molecule 2 is a protein called Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	332	Total	C	N	O	S	0	0	0
			2560	1606	437	507	10			
2	B	332	Total	C	N	O	S	0	0	0
			2572	1614	439	509	10			
2	G	329	Total	C	N	O	S	0	0	0
			2538	1593	431	504	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	SER	THR	CONFLICT	UNP P46828
A	105	GLN	GLU	CONFLICT	UNP P46828
A	320	GLU	GLN	CONFLICT	UNP P46828
B	87	SER	THR	CONFLICT	UNP P46828
B	105	GLN	GLU	CONFLICT	UNP P46828
B	320	GLU	GLN	CONFLICT	UNP P46828
G	87	SER	THR	CONFLICT	UNP P46828
G	105	GLN	GLU	CONFLICT	UNP P46828
G	320	GLU	GLN	CONFLICT	UNP P46828

- Molecule 3 is a protein called HPr-like protein crh.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	W	84	Total 652	C 407	N 109	O 132	P 1	S 3	0	0	0
3	P	84	Total 652	C 407	N 109	O 132	P 1	S 3	0	0	0
3	J	84	Total 652	C 407	N 109	O 132	P 1	S 3	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	33	ILE	VAL	CONFLICT	UNP O06976
W	55	ILE	VAL	CONFLICT	UNP O06976
W	61	ILE	VAL	CONFLICT	UNP O06976
P	33	ILE	VAL	CONFLICT	UNP O06976
P	55	ILE	VAL	CONFLICT	UNP O06976
P	61	ILE	VAL	CONFLICT	UNP O06976
J	33	ILE	VAL	CONFLICT	UNP O06976
J	55	ILE	VAL	CONFLICT	UNP O06976
J	61	ILE	VAL	CONFLICT	UNP O06976

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total 1	I 1	0	0
4	G	2	Total 2	I 2	0	0
4	B	3	Total 3	I 3	0	0
4	A	4	Total 4	I 4	0	0
4	O	1	Total 1	I 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	B	9	Total 9	O 9	0	0
5	G	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	6	Total 6	O 6	0	0
5	P	2	Total 2	O 2	0	0
5	T	1	Total 1	O 1	0	0
5	W	6	Total 6	O 6	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 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: DNA recognition strand CRE

Chain O:

• Molecule 1: DNA recognition strand CRE

Chain T:

• Molecule 1: DNA recognition strand CRE

Chain R:

• Molecule 2: Glucose-resistance amylase regulator

Chain A:

R278 L279 S280 T281 M282 V283 R284 P285 Q286 L287 T288 S289 V290 P293 M294 Y295 D296 I297 G298 A299 V300 A301 M302 R303 L304 L305 T306 K307 Y308 M309 D315 S316 S317 I318 V319 E320 L321 P322 H323 R324 I325 E326 F327 R328 Q329 S330 T331 K332

• Molecule 2: Glucose-resistance amylase regulator

Chain B:

M1 T4 I5 Y6 D7 R10 E11 A12 S13 V14 S15 M16 A17 T18 V19 V22 G25 N26 P27 N28 V29 K30 T33 R34 K35 K36 V37 L38 E39 T40 I41 E42 Y46 R47 P48 N49 A50 L55 K58 K59 T60 T61 T62 V65 I66 I67 P68 D69 I70 S71 N72

I73 F74 Y75 L78 A79 R80 G81 I82 E83 D84 M88 Y89 K90 I94 L95 S96 N97 S98 D99 Q100 N101 K104 Q105 L106 H107 L108 L109 N110 N111 M112 L113 S124 V127 H131 V132 E133 E134 L135 K136 K137 S138 P139 V140 P141 V142 V143

L144 A145 A146 S147 I148 T151 N152 Q153 I154 P155 S156 V157 T158 I159 D160 Y161 E162 Q163 F166 D167 A168 V169 Q170 S171 L172 I173 I180 A181 F182 G185 T186 L187 E188 E189 P190 I191 N192 H193 A194 K195 K196 V197 K198 G199 Y200 K201 R202 A203 L204 T205 L209 P210 V211 R212 D213
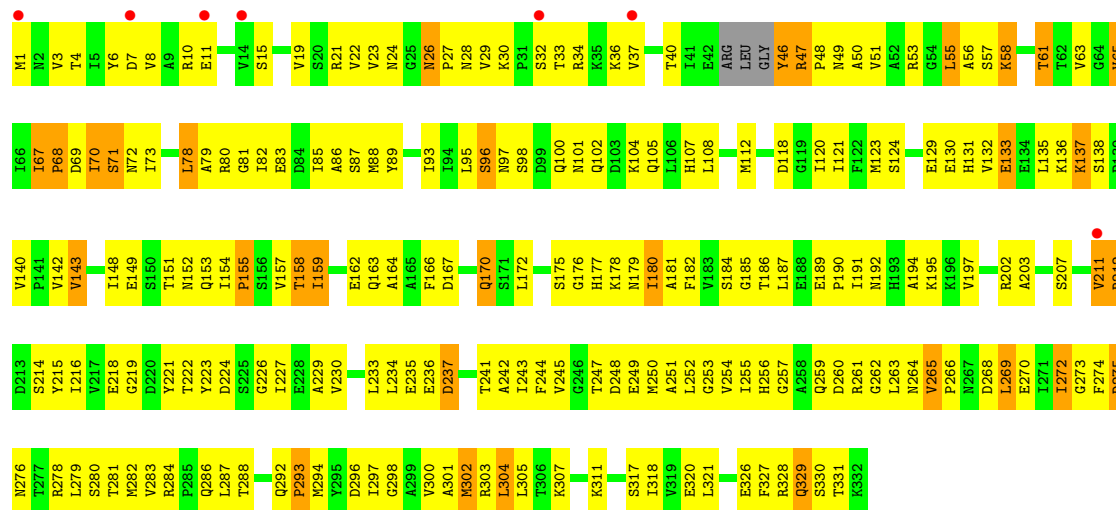
S214 Y215 I216 V217 E218 G219 D220 Y221 T222 Y223 D224 S225 G226 I227 E228 A229 V230 E231 K232 L233 L234 E235 E236 D237 E238 A242 I243 F244 V245 G246 T247 D248 E249 M250 A251 L252 G253 V254 I255 H256 G257 A258 Q259 D260 R261 G262 L263 N264 V265 P266 N267 D268 L269 E270 I271 I272 G273 F274 D275

N276 T277 R278 L279 S280 T281 M282 V283 R284 P285 Q286 L287 T288 S289 V290 P293 M294 Y295 D296 I297 G298 A301 M302 R303 L304 L305 T306 K307 Y308 M309 N310 K311 V314 D315 S316 S317 I318 V319 E320 L321 P322 H323 R324 I325 E326 F327 R328 Q329 S330 T331 K332

• Molecule 2: Glucose-resistance amylase regulator

Chain G:

M1 N2 V3 T4 I5 Y6 D7 V8 A9 R10 E11 V14 S15 V19 S20 R21 V22 V23 N24 G25 N26 P27 N28 V29 K30 P31 S32 T33 R34 K35 K36 V37 T40 I41 E42 ARG LEU GLY Y46 R47 P48 N49 A50 V51 A52 R53 G54 L55 A56 S57 K58 T61 T62 V63 G64 V65

I66 I67 P68 D69 I70 S71 N72 I73 L78 A79 R80 G81 I82 E83 D84 I85 A86 S87 M88 Y89 I93 I94 L95 S96 N97 S98 D99 Q100 N101 Q102 D103 K104 Q105 L106 H107 L108 M112 D118 G119 I120 I121 F122 M123 S124 E129 E130 H131 V132 E133 E134 L135 K136 K137 S138 P139

V140 P141 V142 V143 I148 E149 S150 T151 N152 Q153 I154 P155 S156 V157 T158 I159 E162 Q163 A164 A165 F166 D167 Q170 S171 L172 S175 G176 H177 K178 N179 I180 A181 F182 V183 S184 G185 T186 L187 E188 E189 P190 I191 N192 H193 A194 K195 K196 V197 R202 A203 S207 V211 R212

D213 S214 Y215 I216 V217 E218 G219 D220 Y221 T222 Y223 D224 S225 G226 I227 E228 A229 V230 L233 L234 E235 E236 D237 T241 A242 I243 F244 V245 G246 T247 D248 E249 M250 A251 L252 G253 V254 I255 H256 G257 A258 Q259 D260 R261 G262 L263 N264 V265 P266 N267 D268 L269 E270 I271 I272 G273 F274 D275
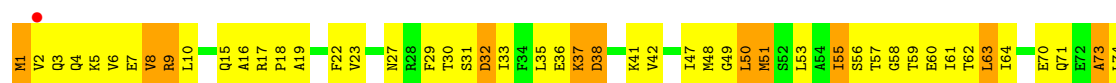
N276 T277 R278 L279 S280 T281 M282 V283 R284 P285 Q286 L287 T288 Q292 P293 M294 Y295 D296 I297 G298 A299 V300 A301 M302 R303 L304 L305 T306 K307 K311 S317 I318 V319 E320 L321 E326 F327 R328 Q329 S330 T331 K332
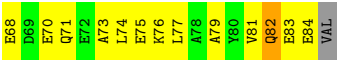
• Molecule 3: HPr-like protein crh

Chain W:

M1 V2 Q3 Q4 K5 V6 E7 V8 R9 L10 Q15 A16 R17 P18 A19 F22 V23 N27 R28 F29 T30 S31 D32 I33 F34 L35 E36 K37 D38 K41 V42 I47 M48 G49 L50 M51 S52 L53 A54 I55 S56 T57 G58 T59 E60 I61 T62 L63 I64 E70 Q71 E72 A73 L74

E75 K76 L77 A78 A79 Y80 V81 Q82 E83 E84 VAL

• Molecule 3: HPr-like protein crh

Chain P:

28% 60% 9% ••

M1 V2 Q3 Q4 K5 V6 E7 V8 R9 L10 K11 T12 A16 R17 P18 L21 F22 V23 Q24 E25 A26 N27 R28 F29 D32 I33 F34 L35 E36 K37 D38 G39 K40 K41 V42 N43 A44 K45 S46 I47 M48 G49 L50 L53 A54 I55 T59 E60 I61 T62 L63 I64 A65 Q66 G67

E68 D69 E70 Q71 E72 A73 L74 E75 K76 L77 A78 A79 Y80 V81 Q82 E83 E84 VAL

• Molecule 3: HPr-like protein crh

Chain J:

35% 52% 11% ••

M1 V2 Q3 Q4 K5 V6 E7 V8 R9 L10 L14 Q15 A16 R17 P18 A19 F22 V23 Q24 E25 F29 T30 S31 D32 L35 E36 K37 K40 K41 V42 N43 A44 K45 S46 I47 M48 G49 L50 M51 S52 L53 A54 I55 T59 E60 I61 T62 L63 I64 A65 Q66 G67 E68 D69

E70 A73 L74 L77 A78 A79 Y80 V81 Q82 E83 E84 VAL

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	83.69Å 158.10Å 125.47Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	79.05 – 2.98 79.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.2 (79.05-2.98) 91.6 (79.05-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.298 0.226 , 0.293	Depositor DCC
R_{free} test set	2450 reflections (8.74%)	DCC
Wilson B-factor (Å^2)	68.9	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 71.7	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10661	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, 0.333 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: IOD, SEP

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	O	0.53	0/366	0.77	0/563
1	R	0.53	0/366	0.83	0/563
1	T	0.51	0/366	0.75	0/563
2	A	0.43	0/2596	0.70	0/3513
2	B	0.46	0/2610	0.76	1/3536 (0.0%)
2	G	0.46	0/2574	0.72	0/3484
3	J	0.54	0/645	0.75	0/863
3	P	0.44	0/645	0.72	0/863
3	W	0.57	0/645	0.83	1/863 (0.1%)
All	All	0.47	0/10813	0.74	2/14811 (0.0%)

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
2	G	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	63	LEU	CA-CB-CG	6.79	130.92	115.30
2	B	187	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	46	TYR	Sidechain

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	O	326	0	181	38	0
1	R	326	0	181	25	0
1	T	326	0	181	25	0
2	A	2560	0	2580	277	0
2	B	2572	0	2602	259	0
2	G	2538	0	2557	249	0
3	J	652	0	668	72	0
3	P	652	0	668	86	0
3	W	652	0	668	80	0
4	A	4	0	0	2	0
4	B	3	0	0	0	0
4	G	2	0	0	3	0
4	O	1	0	0	0	0
4	P	1	0	0	1	0
5	A	10	0	0	0	0
5	B	9	0	0	0	0
5	G	12	0	0	1	0
5	O	6	0	0	0	0
5	P	2	0	0	0	0
5	T	1	0	0	0	0
5	W	6	0	0	0	0
All	All	10661	0	10286	1074	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 51.

The worst 5 of 1074 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)
2:G:288:THR:HG22	2:G:328:ARG:H	1.08	1.09
3:J:9:ARG:HD2	3:J:82:GLN:NE2	1.69	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:183:VAL:HB	2:A:245:VAL:HG12	1.37	1.06
2:B:230:VAL:HG22	2:B:254:VAL:HG13	1.37	1.05
2:A:288:THR:HG22	2:A:328:ARG:H	0.91	1.04

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	
2	A	330/332 (99%)	261 (79%)	54 (16%)	15 (4%)	3	15
2	B	330/332 (99%)	257 (78%)	61 (18%)	12 (4%)	4	20
2	G	325/332 (98%)	242 (74%)	69 (21%)	14 (4%)	3	16
3	J	81/85 (95%)	56 (69%)	19 (24%)	6 (7%)	1	5
3	P	81/85 (95%)	54 (67%)	23 (28%)	4 (5%)	2	14
3	W	81/85 (95%)	65 (80%)	13 (16%)	3 (4%)	4	20
All	All	1228/1251 (98%)	935 (76%)	239 (20%)	54 (4%)	3	16

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	28	ASN
2	B	28	ASN
2	B	275	ASP
3	P	38	ASP
2	G	27	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	
2	A	285/289 (99%)	249 (87%)	36 (13%)	5	21
2	B	289/289 (100%)	256 (89%)	33 (11%)	7	25
2	G	284/289 (98%)	248 (87%)	36 (13%)	5	21
3	J	68/69 (99%)	60 (88%)	8 (12%)	6	24
3	P	68/69 (99%)	61 (90%)	7 (10%)	8	30
3	W	68/69 (99%)	58 (85%)	10 (15%)	3	15
All	All	1062/1074 (99%)	932 (88%)	130 (12%)	6	23

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	143	VAL
2	B	284	ARG
2	G	311	LYS
2	B	188	GLU
2	B	215	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	97	ASN
2	B	170	GLN
2	G	152	ASN
2	B	152	ASN
2	A	193	HIS

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	SEP	J	46	3	9,9,10	1.24	1 (11%)	9,12,14	1.73	2 (22%)
3	SEP	P	46	3	9,9,10	0.99	0	9,12,14	1.97	2 (22%)
3	SEP	W	46	3	9,9,10	0.93	0	9,12,14	1.64	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	J	46	3	-	0/5/8/10	0/0/0/0
3	SEP	P	46	3	-	0/5/8/10	0/0/0/0
3	SEP	W	46	3	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	46	SEP	CA-C	2.40	1.53	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	46	SEP	OG-CB-CA	2.21	110.35	108.17
3	W	46	SEP	O3P-P-O1P	3.02	122.32	110.50
3	J	46	SEP	O3P-P-O1P	3.03	122.34	110.50
3	P	46	SEP	O3P-P-O1P	3.21	123.05	110.50
3	J	46	SEP	OG-CB-CA	3.66	111.78	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	46	SEP	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 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 ⓘ

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	O	16/16 (100%)	-0.66	0	100	100	33, 82, 107, 108	0
1	R	16/16 (100%)	-0.36	1 (6%)	21	11	32, 78, 135, 151	0
1	T	16/16 (100%)	-0.63	0	100	100	50, 72, 119, 137	0
2	A	332/332 (100%)	-0.35	3 (0%)	84	67	25, 72, 106, 137	0
2	B	332/332 (100%)	-0.23	3 (0%)	84	67	25, 63, 100, 125	0
2	G	329/332 (99%)	-0.20	7 (2%)	64	43	15, 63, 117, 144	0
3	J	83/85 (97%)	-0.34	0	100	100	23, 60, 80, 115	0
3	P	83/85 (97%)	-0.39	0	100	100	38, 72, 92, 119	0
3	W	83/85 (97%)	-0.49	2 (2%)	59	38	32, 58, 77, 110	0
All	All	1290/1299 (99%)	-0.30	16 (1%)	79	59	15, 65, 107, 151	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	11	GLU	4.2
2	G	32	SER	4.1
2	B	1	MET	3.7
2	G	7	ASP	3.5
2	G	211	VAL	3.4

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
3	SEP	J	46	10/11	0.98	0.13	-	22,33,37,40	0
3	SEP	P	46	10/11	0.97	0.12	-	49,56,58,59	0
3	SEP	W	46	10/11	0.98	0.13	-	23,39,49,49	0

6.3   Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4   Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
4	IOD	G	414	1/1	0.98	0.23	2.91	45,45,45,45	1
4	IOD	B	420	1/1	0.92	0.12	-1.15	110,110,110,110	1
4	IOD	B	419	1/1	0.96	0.11	-2.05	109,109,109,109	1
4	IOD	A	411	1/1	0.88	0.07	-	120,120,120,120	1
4	IOD	A	410	1/1	0.90	0.07	-	77,77,77,77	1
4	IOD	B	422	1/1	0.88	0.07	-	114,114,114,114	1
4	IOD	A	413	1/1	0.99	0.05	-	66,66,66,66	1
4	IOD	A	412	1/1	0.91	0.09	-	95,95,95,95	1
4	IOD	P	421	1/1	0.96	0.09	-	99,99,99,99	1
4	IOD	O	415	1/1	0.87	0.06	-	111,111,111,111	1
4	IOD	G	418	1/1	0.97	0.13	-	98,98,98,98	1

6.5   Other polymers ⓘ

There are no such residues in this entry.

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