



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 5, 2017 – 12:14 AM EST

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)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

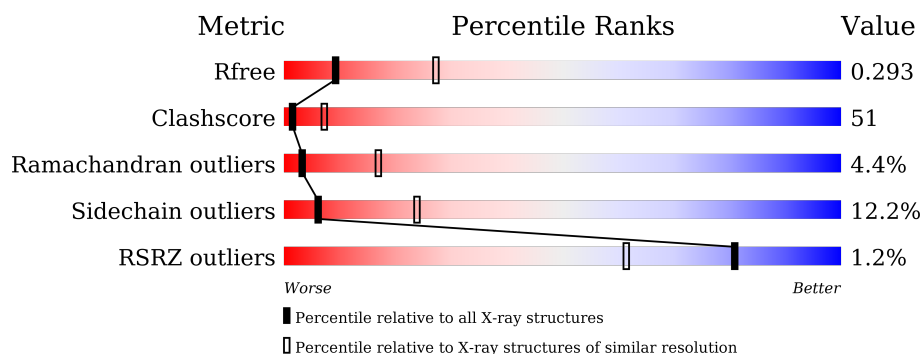
# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (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  $\geq 3$ , 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	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% .

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	J	85	
3	P	85	
3	W	85	

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

*Continued on next page...*

*Continued from previous page...*

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 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: DNA recognition strand CRE

Chain O:  100%

C700  
T701  
G702  
A703  
A704  
A705  
G706  
C707  
G708  
C709  
T710  
T711  
A712  
C713  
A714  
G715

- Molecule 1: DNA recognition strand CRE

Chain T:  100%

C700  
T701  
G702  
A703  
A704  
A705  
G706  
C707  
G708  
C709  
T710  
T711  
A712  
C713  
A714  
G715

- Molecule 1: DNA recognition strand CRE

Chain R:  6% 100%

C700  
T701  
G702  
A703  
A704  
A705  
G706  
C707  
G708  
C709  
T710  
T711  
A712  
C713  
A714  
G715

- Molecule 2: Glucose-resistance amylase regulator

Chain A:  33% 56% 11%

M1  
M2  
V3  
T4  
I5  
Y6  
D7  
V8  
A9  
R10  
E11  
A12  
S13  
V14  
S15  
M16  
A17  
T18  
V19  
S20  
R21  
V22  
V23  
M28  
V29  
K30  
P31  
S32  
T33  
R34  
K35  
K36  
V37  
L38  
E39  
T40  
R43  
L44  
F122  
M123  
L124  
K128  
K129  
T60  
T61  
V65  
I66  
I67  
P68  
D69  
I70  
S71  
N72  
I73  
F74  
Y75  
A76

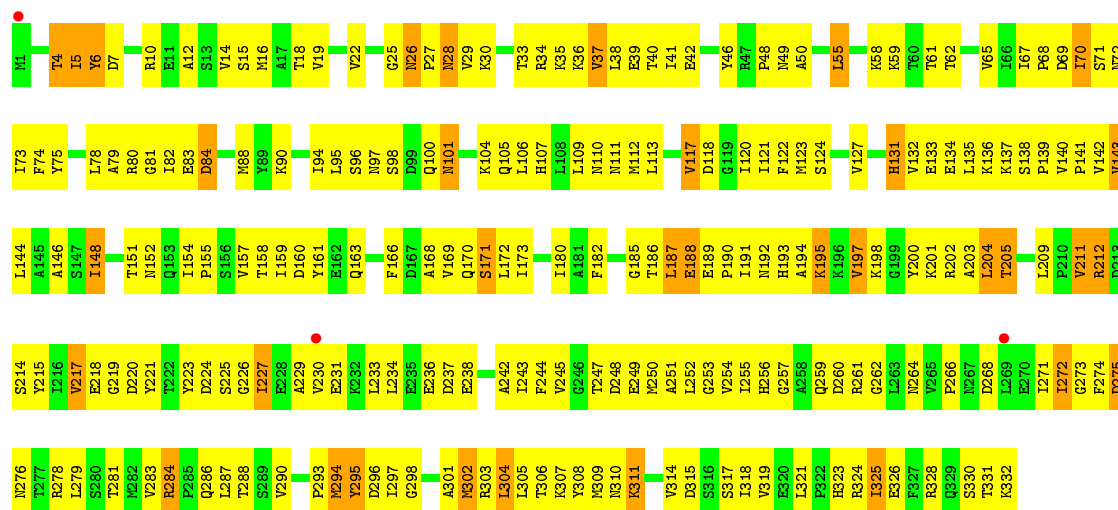
E77  
L78  
A79  
S150  
R80  
T81  
G81  
I82  
E83  
D84  
T85  
A86  
Y89  
N92  
I93  
T94  
L95  
A96  
S96  
N97  
S98  
D99  
Q100  
V101  
N101  
Q102  
D103  
K104  
Q105  
L106  
L109  
N110  
N110  
L113  
G114  
K115  
Q116  
V117  
D118  
T121  
F122  
M123  
S124  
T128  
E129  
H130  
H131  
V132  
E133  
E134  
L135  
P139  
V140  
V143  
L144  
A145  
A146

S147  
I148  
E149  
S150  
T151  
N152  
Q153  
T154  
P155  
S156  
V157  
T158  
I159  
D160  
Y161  
E162  
Q163  
A164  
A165  
F166  
D167  
A168  
V169  
Q170  
S171  
D174  
S175  
G176  
H177  
K178  
H179  
I180  
A181  
F182  
V183  
E188  
E189  
P190  
I191  
N192  
H193  
A194  
K195  
K196  
V197  
K198  
G199  
Y200  
K201  
R202  
E206  
S207  
V211  
R212  
D213  
N216  
S214

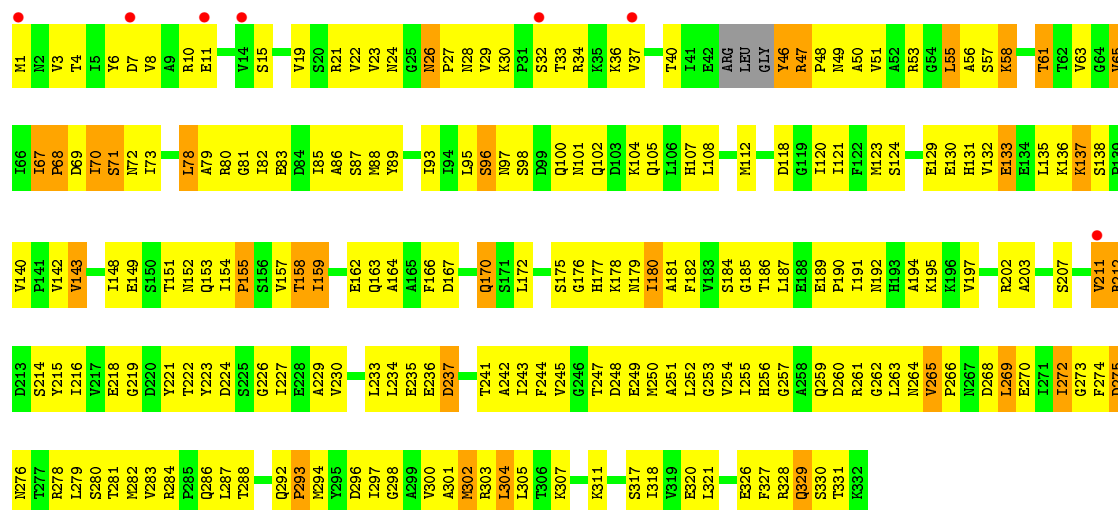
Y215  
I216  
V217  
E218  
G219  
D220  
Y221  
T222  
Y223  
D224  
S225  
G226  
D227  
E228  
A229  
V230  
E231  
K232  
L233  
L234  
E235  
E236  
D237  
V238  
E239  
P240  
T241  
A242  
L243  
F244  
G245  
G246  
T247  
M250  
A251  
L252  
G253  
V254  
E256  
G257  
E261  
G262  
L263  
M264  
V265  
P266  
N267  
D268  
L269  
E270  
I271  
L272  
G273  
F274  
D275  
N276  
T277



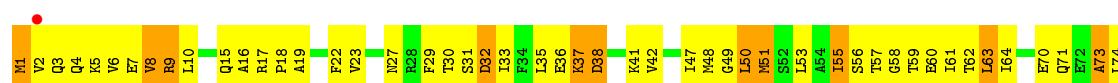
• Molecule 2: Glucose-resistance amylase regulator



• Molecule 2: Glucose-resistance amylase regulator



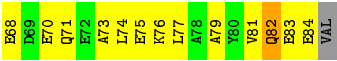
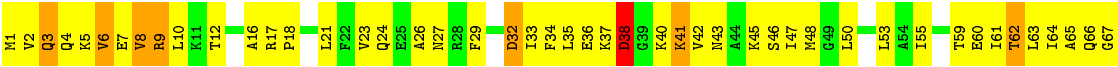
• Molecule 3: HPr-like protein crh



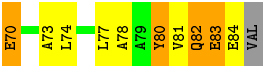
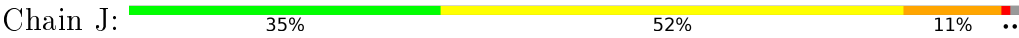




• Molecule 3: HPr-like protein crh



• Molecule 3: HPr-like protein crh



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	68.9	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 71.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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 ⓘ

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

*Continued on next page...*

*Continued from previous page...*

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 [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	
2	A	330/332 (99%)	261 (79%)	54 (16%)	15 (4%)	3	16
2	B	330/332 (99%)	257 (78%)	61 (18%)	12 (4%)	4	22
2	G	325/332 (98%)	242 (74%)	69 (21%)	14 (4%)	3	18
3	J	81/85 (95%)	56 (69%)	19 (24%)	6 (7%)	1	6
3	P	81/85 (95%)	54 (67%)	23 (28%)	4 (5%)	3	15
3	W	81/85 (95%)	65 (80%)	13 (16%)	3 (4%)	4	21
All	All	1228/1251 (98%)	935 (76%)	239 (20%)	54 (4%)	3	17

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 ⓘ

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	22
2	B	289/289 (100%)	256 (89%)	33 (11%)	7	27
2	G	284/289 (98%)	248 (87%)	36 (13%)	5	22
3	J	68/69 (99%)	60 (88%)	8 (12%)	6	25
3	P	68/69 (99%)	61 (90%)	7 (10%)	9	31
3	W	68/69 (99%)	58 (85%)	10 (15%)	4	16
All	All	1062/1074 (99%)	932 (88%)	130 (12%)	6	24

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 ⓘ

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	7,9,10	1.12	0	8,12,14	2.10	2 (25%)
3	SEP	P	46	3	7,9,10	1.04	0	8,12,14	2.32	3 (37%)
3	SEP	W	46	3	7,9,10	1.07	1 (14%)	8,12,14	1.95	4 (50%)

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	W	46	SEP	P-O3P	-2.12	1.47	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	46	SEP	O2P-P-O1P	-2.32	103.06	110.63
3	W	46	SEP	O-C-CA	-2.15	119.96	125.72
3	W	46	SEP	O2P-P-O1P	-2.00	104.09	110.63
3	W	46	SEP	OG-CB-CA	2.39	110.35	108.26
3	W	46	SEP	O3P-P-O1P	3.58	122.32	110.63

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	O	16/16 (100%)	-0.66	0 <span>100</span> <span>100</span>	33, 82, 107, 108	0
1	R	16/16 (100%)	-0.36	1 (6%) <span>23</span> <span>11</span>	32, 78, 135, 151	0
1	T	16/16 (100%)	-0.63	0 <span>100</span> <span>100</span>	50, 72, 119, 137	0
2	A	332/332 (100%)	-0.35	3 (0%) <span>85</span> <span>69</span>	25, 72, 106, 137	0
2	B	332/332 (100%)	-0.23	3 (0%) <span>85</span> <span>69</span>	25, 63, 100, 125	0
2	G	329/332 (99%)	-0.20	7 (2%) <span>67</span> <span>44</span>	15, 63, 117, 144	0
3	J	83/85 (97%)	-0.34	0 <span>100</span> <span>100</span>	23, 60, 80, 115	0
3	P	83/85 (97%)	-0.39	0 <span>100</span> <span>100</span>	38, 72, 92, 119	0
3	W	83/85 (97%)	-0.49	2 (2%) <span>62</span> <span>39</span>	32, 58, 77, 110	0
All	All	1290/1299 (99%)	-0.30	16 (1%) <span>81</span> <span>61</span>	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	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 [i](#)

There are no carbohydrates 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. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	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 [i](#)

There are no such residues in this entry.