



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:47 PM GMT

PDB ID : 4A0S  
Title : STRUCTURE OF THE 2-OCTENOYL-COA CARBOXYLASE REDUCTASE CINF IN COMPLEX WITH NADP AND 2-OCTENOYL-COA  
Authors : Quade, N.; Huo, L.; Rachid, S.; Heinz, D.W.; Muller, R.  
Deposited on : 2011-09-12  
Resolution : 1.90 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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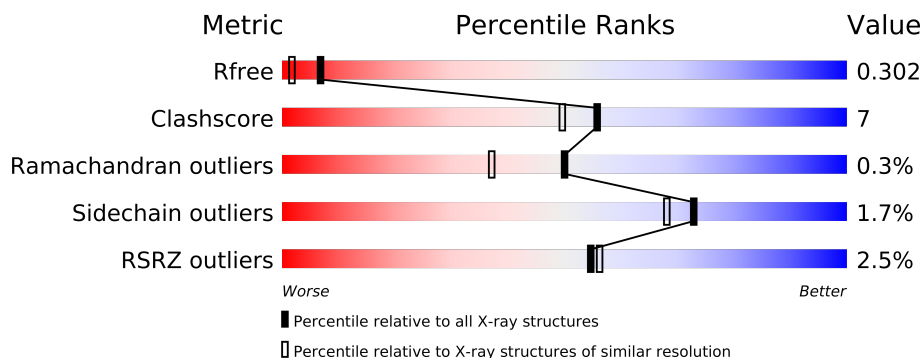
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	447	
1	B	447	
1	C	447	
1	D	447	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CO8	C	1446	-	X
2	CO8	D	1446	-	X

## 2 Entry composition i

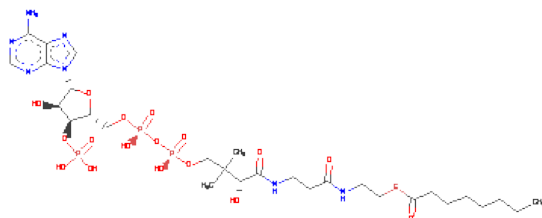
There are 4 unique types of molecules in this entry. The entry contains 15766 atoms, of which 0 are hydrogen and 0 are deuterium.

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 OCTENOYL-COA REDUCTASE/CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	3	0
			3375	2115	613	631	16			
1	B	445	Total	C	N	O	S	0	2	0
			3371	2112	615	628	16			
1	C	444	Total	C	N	O	S	0	2	0
			3360	2106	609	629	16			
1	D	444	Total	C	N	O	S	0	0	0
			3348	2098	608	626	16			

- Molecule 2 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: C<sub>29</sub>H<sub>50</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



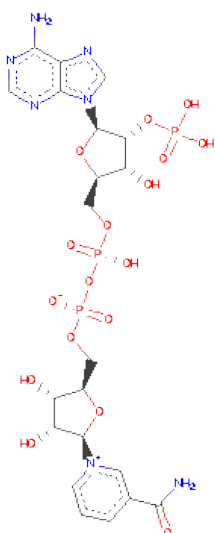
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			57	29	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			57	29	7	17	3 1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	522	Total	O	0	0
			522	522		
4	B	482	Total	O	0	0
			482	482		
4	C	457	Total	O	0	0
			457	457		

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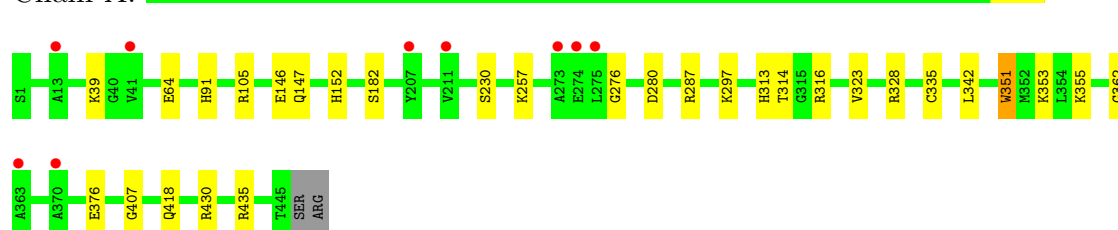
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	431	Total 431	O 431	0	0

### 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.

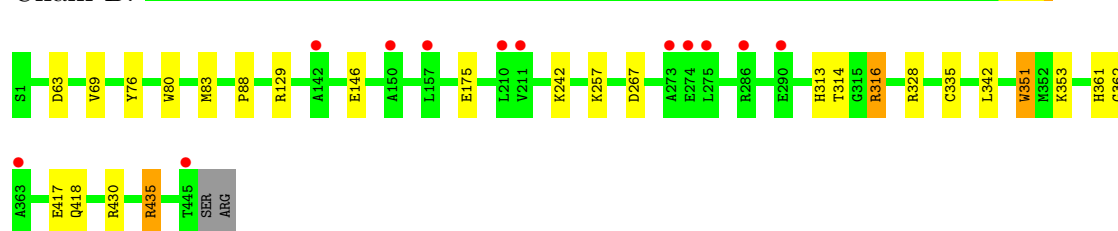
#### • Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain A:



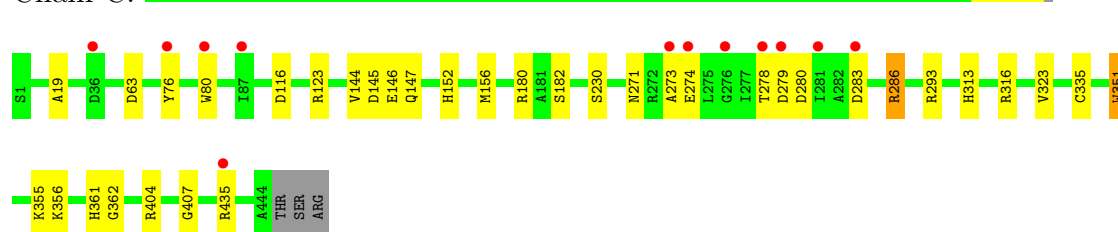
#### • Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain B:



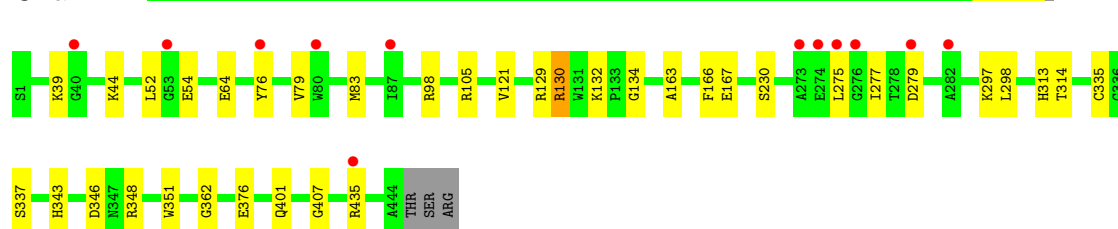
#### • Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain C:



#### • Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.01Å 83.30Å 122.74Å 90.00° 110.96° 90.00°	Depositor
Resolution (Å)	47.21 – 1.90 47.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.21-1.90) 98.9 (47.21-1.90)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.199 , 0.250 0.256 , 0.302	Depositor DCC
$R_{free}$ test set	7037 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 1.4	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 140723 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO8, NAP

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	0.53	0/3452	0.66	0/4687
1	B	0.54	0/3445	0.67	0/4677
1	C	0.52	0/3434	0.67	0/4663
1	D	0.51	0/3416	0.68	3/4639 (0.1%)
All	All	0.53	0/13747	0.67	3/18666 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	275	LEU	CA-CB-CG	5.06	126.93	115.30
1	D	130	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3375	0	0	20	0
1	B	3371	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3360	0	0	25	0
1	D	3348	0	0	21	0
2	A	57	0	46	2	0
2	B	57	0	46	4	0
2	C	57	0	46	4	0
2	D	57	0	46	4	0
3	A	48	0	25	5	0
3	B	48	0	25	8	0
3	C	48	0	25	6	0
3	D	48	0	25	4	0
4	A	522	0	0	5	0
4	B	482	0	0	8	0
4	C	457	0	0	3	0
4	D	431	0	0	7	0
All	All	15766	0	284	93	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (93) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:362:GLY:N	3:B:1446:NAP:H72N	1.71	0.87
1:C:145:ASP:OD2	1:D:130:ARG:NH2	2.09	0.85
4:A:2380:HOH:O	2:D:1446:CO8:O4A	2.01	0.77
1:D:362:GLY:N	3:D:1445:NAP:H72N	1.83	0.76
1:A:362:GLY:N	3:A:1447:NAP:H72N	1.87	0.73
1:D:297:LYS:NZ	4:D:2297:HOH:O	2.21	0.72
1:C:362:GLY:N	3:C:1445:NAP:H72N	1.89	0.71
1:C:63:ASP:OD2	4:C:2120:HOH:O	2.12	0.67
1:D:79:VAL:CG1	1:D:83:MET:CE	2.73	0.67
1:D:376:GLU:OE1	4:D:2347:HOH:O	2.14	0.66
2:B:1447:CO8:O7A	1:C:286:ARG:NH2	2.29	0.65
1:B:417:GLU:OE2	4:B:2438:HOH:O	2.14	0.65
1:A:376:GLU:OE2	4:A:2276:HOH:O	2.14	0.65
1:A:280:ASP:OD1	1:A:287[A]:ARG:NH2	2.32	0.63
1:B:80:TRP:CE3	1:B:83:MET:CE	2.83	0.62
1:B:362:GLY:N	3:B:1446:NAP:N7N	2.45	0.61
4:B:2261:HOH:O	1:C:356:LYS:NZ	2.34	0.60
1:B:63:ASP:OD2	4:B:2102:HOH:O	2.16	0.58
1:B:435:ARG:NH1	4:B:2467:HOH:O	2.37	0.57
1:B:335:CYS:O	3:B:1446:NAP:H2N	2.04	0.57
1:A:335:CYS:O	3:A:1447:NAP:H2N	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:1446:NAP:C7N	2:B:1447:CO8:H2'1	2.36	0.55
1:D:335:CYS:O	3:D:1445:NAP:H2N	2.07	0.55
1:C:335:CYS:O	3:C:1445:NAP:H2N	2.07	0.55
3:B:1446:NAP:H3B	3:B:1446:NAP:H8A	1.89	0.54
1:C:404:ARG:NH2	4:C:2092:HOH:O	2.40	0.54
1:A:257:LYS:NZ	3:A:1447:NAP:O3X	2.41	0.54
1:D:52:LEU:N	4:D:2077:HOH:O	2.42	0.52
1:D:166:PHE:CE2	2:D:1446:CO8:H32	2.45	0.52
1:B:430:ARG:NH1	4:B:2459:HOH:O	2.45	0.50
1:C:271:ASN:O	1:C:274:GLU:CB	2.60	0.50
1:C:362:GLY:N	3:C:1445:NAP:N7N	2.59	0.49
1:C:76:TYR:CE1	1:C:80:TRP:NE1	2.80	0.49
1:D:230:SER:O	1:D:407:GLY:N	2.46	0.49
1:A:276:GLY:O	1:A:287[B]:ARG:NH2	2.46	0.48
1:C:146:GLU:OE2	1:C:182:SER:OG	2.31	0.48
1:A:418:GLN:NE2	4:A:2487:HOH:O	2.46	0.48
1:B:242:LYS:NZ	4:B:2280:HOH:O	2.46	0.48
1:C:323:VAL:O	1:C:355:LYS:NZ	2.47	0.47
1:B:316:ARG:NH1	1:B:342:LEU:O	2.48	0.47
1:A:146[A]:GLU:OE2	1:A:182:SER:OG	2.33	0.47
1:B:257:LYS:NZ	3:B:1446:NAP:O2X	2.47	0.47
3:A:1447:NAP:H8A	3:A:1447:NAP:H3B	1.98	0.46
1:A:91:HIS:NE2	2:A:1446:CO8:O2A	2.48	0.46
1:D:121:VAL:O	1:D:134:GLY:N	2.49	0.46
1:B:353:LYS:NZ	2:C:1446:CO8:H121	2.31	0.46
3:C:1445:NAP:H52N	3:C:1445:NAP:H52A	1.97	0.46
1:D:362:GLY:N	3:D:1445:NAP:N7N	2.59	0.45
1:D:376:GLU:OE2	4:D:2207:HOH:O	2.21	0.45
1:A:147[A]:GLN:OE1	1:B:129:ARG:N	2.49	0.45
1:D:64:GLU:OE1	1:D:105:ARG:NH1	2.50	0.45
1:A:230:SER:O	1:A:407:GLY:N	2.50	0.45
1:C:147[A]:GLN:OE1	1:D:129:ARG:N	2.50	0.45
2:A:1446:CO8:H2'1	3:A:1447:NAP:C7N	2.47	0.44
1:C:273:ALA:O	1:C:274:GLU:C	2.55	0.44
1:D:44:LYS:O	1:D:401:GLN:NE2	2.51	0.44
1:C:361:HIS:CE1	2:C:1446:CO8:H5'1	2.53	0.44
1:B:267:ASP:CB	4:B:2307:HOH:O	2.64	0.44
1:D:163:ALA:N	1:D:167:GLU:OE1	2.51	0.44
1:B:146:GLU:N	1:B:146:GLU:OE1	2.50	0.44
3:C:1445:NAP:C7N	2:C:1446:CO8:H2'1	2.48	0.43
1:B:418:GLN:NE2	4:B:2442:HOH:O	2.51	0.43
1:C:351:TRP:C	1:C:351:TRP:CD1	2.91	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:361:HIS:CE1	2:B:1447:CO8:H5'1	2.54	0.43
3:C:1445:NAP:C4N	2:C:1446:CO8:H3'2	2.49	0.43
3:B:1446:NAP:C3B	3:B:1446:NAP:H8A	2.49	0.42
1:A:323:VAL:O	1:A:355:LYS:NZ	2.52	0.42
3:B:1446:NAP:H52A	3:B:1446:NAP:H52N	2.01	0.41
1:A:353:LYS:NZ	2:D:1446:CO8:H121	2.35	0.41
1:D:132:LYS:NZ	4:D:2165:HOH:O	2.53	0.41
1:B:328:ARG:NH2	1:C:156:MET:O	2.53	0.41
1:B:351:TRP:C	1:B:351:TRP:CD1	2.94	0.41
1:D:346:ASP:OD2	1:D:348:ARG:NH2	2.53	0.41
1:B:69:VAL:N	1:B:175:GLU:O	2.53	0.41
1:C:286:ARG:NE	4:C:2313:HOH:O	2.54	0.41
1:A:430:ARG:NH1	4:A:2504:HOH:O	2.53	0.41
3:D:1445:NAP:C7N	2:D:1446:CO8:H2'1	2.50	0.41
2:B:1447:CO8:O4A	1:C:293:ARG:NH2	2.54	0.41
1:C:230:SER:O	1:C:407:GLY:N	2.52	0.41
1:A:351:TRP:CD1	1:A:351:TRP:C	2.94	0.41
1:A:64:GLU:OE2	1:A:105:ARG:NH2	2.54	0.41
1:D:337:SER:OG	1:D:343:HIS:NE2	2.54	0.41
1:D:54:GLU:N	4:D:2080:HOH:O	2.54	0.41
1:C:283:ASP:OD1	1:C:316:ARG:NH2	2.54	0.41
1:D:98:ARG:NH1	4:D:2131:HOH:O	2.53	0.41
1:A:328:ARG:N	4:A:2395:HOH:O	2.54	0.41
1:C:144:VAL:O	1:C:180:ARG:NH1	2.54	0.40
1:A:316:ARG:NH1	1:A:342:LEU:O	2.55	0.40
1:C:278:THR:OG1	1:C:280:ASP:OD1	2.40	0.40
1:C:146:GLU:O	1:C:152:HIS:NE2	2.54	0.40
1:C:19:ALA:O	1:C:123:ARG:NH2	2.54	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	446/447 (100%)	433 (97%)	12 (3%)	1 (0%)	56 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	445/447 (100%)	433 (97%)	11 (2%)	1 (0%)	56	44
1	C	444/447 (99%)	429 (97%)	14 (3%)	1 (0%)	56	44
1	D	442/447 (99%)	427 (97%)	13 (3%)	2 (0%)	38	23
All	All	1777/1788 (99%)	1722 (97%)	50 (3%)	5 (0%)	50	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	C	313	HIS
1	D	313	HIS
1	B	313	HIS
1	D	277	ILE

### 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	351/350 (100%)	346 (99%)	5 (1%)	78	75
1	B	350/350 (100%)	344 (98%)	6 (2%)	73	68
1	C	349/350 (100%)	344 (99%)	5 (1%)	78	75
1	D	347/350 (99%)	340 (98%)	7 (2%)	68	61
All	All	1397/1400 (100%)	1374 (98%)	23 (2%)	73	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	297	LYS
1	A	314	THR
1	A	351	TRP
1	A	435	ARG
1	B	76	TYR
1	B	88	PRO

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Mol	Chain	Res	Type
1	B	314	THR
1	B	316	ARG
1	B	351	TRP
1	B	435	ARG
1	C	116	ASP
1	C	279	ASP
1	C	286	ARG
1	C	351	TRP
1	C	435	ARG
1	D	39	LYS
1	D	76	TYR
1	D	279	ASP
1	D	298	LEU
1	D	314	THR
1	D	351	TRP
1	D	435	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 ligands 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	$\# Z  > 2$
2	CO8	A	1446	-	59,59,59	2.12	12 (20%)	85,85,85	1.87	14 (16%)
3	NAP	A	1447	-	52,52,52	1.60	8 (15%)	80,80,80	2.20	21 (26%)
3	NAP	B	1446	-	52,52,52	1.52	8 (15%)	80,80,80	2.08	12 (15%)
2	CO8	B	1447	-	59,59,59	1.93	11 (18%)	85,85,85	1.70	12 (14%)
3	NAP	C	1445	-	52,52,52	1.77	11 (21%)	80,80,80	3.01	20 (25%)
2	CO8	C	1446	-	59,59,59	2.03	10 (16%)	85,85,85	1.73	12 (14%)
3	NAP	D	1445	-	52,52,52	1.95	10 (19%)	80,80,80	3.11	27 (33%)
2	CO8	D	1446	-	59,59,59	1.88	10 (16%)	85,85,85	1.80	15 (17%)

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
2	CO8	A	1446	-	-	0/58/74/74	0/1/3/3
3	NAP	A	1447	-	-	0/35/67/67	0/3/5/5
3	NAP	B	1446	-	-	0/35/67/67	0/3/5/5
2	CO8	B	1447	-	-	0/58/74/74	0/1/3/3
3	NAP	C	1445	-	-	0/35/67/67	0/3/5/5
2	CO8	C	1446	-	-	0/58/74/74	0/1/3/3
3	NAP	D	1445	-	-	0/35/67/67	0/3/5/5
2	CO8	D	1446	-	-	0/58/74/74	0/1/3/3

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1446	CO8	C2'-C1'	-11.07	1.38	1.50
2	B	1447	CO8	C2'-C1'	-10.08	1.39	1.50
2	C	1446	CO8	C2'-C1'	-9.86	1.39	1.50
2	D	1446	CO8	C2'-C1'	-9.83	1.39	1.50
3	D	1445	NAP	PA-O3	7.22	1.72	1.59
3	A	1447	NAP	O4B-C1B	5.79	1.50	1.41
3	D	1445	NAP	PN-O1N	5.55	1.62	1.48
3	C	1445	NAP	PA-O3	5.40	1.69	1.59
3	D	1445	NAP	P2B-O1X	5.04	1.68	1.51
3	C	1445	NAP	PN-O3	4.75	1.70	1.60
2	C	1446	CO8	O4B-C1B	4.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1445	NAP	P2B-O1X	4.47	1.66	1.51
3	B	1446	NAP	O4B-C1B	4.46	1.48	1.41
2	C	1446	CO8	P1A-O3A	4.10	1.67	1.59
3	B	1446	NAP	C4A-N9A	-4.05	1.31	1.37
2	B	1447	CO8	O4B-C1B	4.02	1.47	1.41
3	C	1445	NAP	PN-O1N	4.00	1.58	1.48
3	A	1447	NAP	C4A-N9A	-3.95	1.32	1.37
2	A	1446	CO8	P1A-O1A	3.88	1.66	1.51
2	D	1446	CO8	O4B-C1B	3.86	1.47	1.41
3	D	1445	NAP	O4B-C1B	3.86	1.47	1.41
3	D	1445	NAP	C4A-N9A	-3.79	1.32	1.37
2	C	1446	CO8	P2A-O3A	3.76	1.66	1.59
3	D	1445	NAP	P2B-O2X	3.67	1.68	1.54
3	C	1445	NAP	P2B-O2X	3.65	1.68	1.54
2	A	1446	CO8	C3'-C2'	-3.64	1.38	1.52
2	B	1447	CO8	P1A-O3A	3.63	1.66	1.59
3	A	1447	NAP	P2B-O1X	3.63	1.63	1.51
2	A	1446	CO8	P3B-O7A	3.62	1.63	1.51
2	A	1446	CO8	O4B-C1B	3.55	1.46	1.41
2	B	1447	CO8	C3'-C2'	-3.54	1.38	1.52
3	A	1447	NAP	PN-O1N	3.50	1.57	1.48
2	C	1446	CO8	P3B-O7A	3.45	1.62	1.51
2	D	1446	CO8	P3B-O7A	3.42	1.62	1.51
2	C	1446	CO8	C3'-C2'	-3.29	1.39	1.52
3	B	1446	NAP	C2N-N1N	3.26	1.39	1.35
2	D	1446	CO8	C3'-C2'	-3.25	1.39	1.52
3	C	1445	NAP	P2B-O2B	3.25	1.69	1.59
2	A	1446	CO8	C4A-N9A	-3.24	1.33	1.37
3	C	1445	NAP	C4A-N9A	-3.20	1.33	1.37
2	D	1446	CO8	P1A-O1A	3.18	1.63	1.51
2	B	1447	CO8	P2A-O4A	3.18	1.63	1.51
3	A	1447	NAP	O4D-C1D	3.07	1.46	1.41
2	C	1446	CO8	P2A-O4A	3.00	1.62	1.51
3	D	1445	NAP	P2B-O2B	2.92	1.68	1.59
2	C	1446	CO8	P1A-O1A	2.87	1.62	1.51
2	A	1446	CO8	P3B-O8A	2.84	1.65	1.54
2	A	1446	CO8	P1A-O3A	2.84	1.65	1.59
2	B	1447	CO8	P3B-O9A	2.83	1.65	1.54
2	D	1446	CO8	C4A-N9A	-2.82	1.33	1.37
3	A	1447	NAP	C6N-N1N	2.69	1.43	1.35
2	D	1446	CO8	P1A-O3A	2.65	1.64	1.59
2	D	1446	CO8	P2A-O4A	2.65	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1447	CO8	C4A-N9A	-2.60	1.34	1.37
2	A	1446	CO8	P2A-O3A	2.59	1.64	1.59
3	C	1445	NAP	C2D-C1D	-2.58	1.49	1.53
3	B	1446	NAP	C6N-N1N	2.57	1.42	1.35
3	B	1446	NAP	PN-O1N	2.54	1.55	1.48
3	B	1446	NAP	P2B-O1X	2.53	1.59	1.51
2	A	1446	CO8	OAP-CAP	2.53	1.46	1.42
2	C	1446	CO8	C4A-N9A	-2.45	1.34	1.37
2	A	1446	CO8	O1'-C1'	2.44	1.24	1.21
3	C	1445	NAP	C2N-N1N	2.42	1.38	1.35
2	D	1446	CO8	P2A-O3A	2.42	1.64	1.59
3	D	1445	NAP	PN-O3	2.41	1.65	1.60
3	B	1446	NAP	O4D-C4D	2.40	1.50	1.45
3	A	1447	NAP	C2N-N1N	2.37	1.38	1.35
2	B	1447	CO8	P2A-O3A	2.31	1.64	1.59
2	A	1446	CO8	P2A-O4A	2.29	1.60	1.51
3	D	1445	NAP	C6N-N1N	2.29	1.42	1.35
2	B	1447	CO8	OAP-CAP	2.20	1.46	1.42
3	C	1445	NAP	C6N-N1N	2.13	1.41	1.35
2	D	1446	CO8	P3B-O8A	2.10	1.62	1.54
2	B	1447	CO8	P3B-O8A	2.07	1.62	1.54
3	D	1445	NAP	O4D-C1D	2.07	1.44	1.41
3	A	1447	NAP	C2B-C1B	-2.07	1.49	1.52
3	B	1446	NAP	C5A-N7A	-2.05	1.32	1.40
2	C	1446	CO8	O1'-C1'	2.04	1.24	1.21
3	C	1445	NAP	O4B-C1B	2.03	1.44	1.41
2	B	1447	CO8	O1'-C1'	2.02	1.24	1.21

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1445	NAP	O3X-P2B-O1X	-11.51	72.81	110.44
3	D	1445	NAP	N3A-C2A-N1A	-11.25	119.31	128.71
3	B	1446	NAP	N3A-C2A-N1A	-9.73	120.57	128.71
3	A	1447	NAP	O4D-C1D-N1N	-9.51	98.22	107.95
3	D	1445	NAP	O3X-P2B-O2X	-9.46	70.78	107.61
3	C	1445	NAP	N3A-C2A-N1A	-9.17	121.04	128.71
2	A	1446	CO8	N3A-C2A-N1A	-8.95	121.22	128.71
3	C	1445	NAP	O2N-PN-O3	-8.85	84.94	108.79
2	C	1446	CO8	N3A-C2A-N1A	-8.80	121.35	128.71
2	B	1447	CO8	N3A-C2A-N1A	-8.79	121.36	128.71
2	D	1446	CO8	N3A-C2A-N1A	-8.58	121.53	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1445	NAP	O3-PN-O1N	-8.37	88.83	108.83
3	B	1446	NAP	O4D-C1D-N1N	-8.36	99.40	107.95
3	D	1445	NAP	O2N-PN-O3	-8.30	86.42	108.79
3	D	1445	NAP	O3X-P2B-O2B	-8.26	83.31	107.09
3	A	1447	NAP	N3A-C2A-N1A	-7.80	122.19	128.71
3	D	1445	NAP	O3X-P2B-O1X	-7.42	86.19	110.44
3	C	1445	NAP	O3X-P2B-O2B	-7.41	85.75	107.09
3	C	1445	NAP	O3-PN-O1N	-7.13	91.79	108.83
3	C	1445	NAP	O3X-P2B-O2X	-7.08	80.03	107.61
2	A	1446	CO8	C3'-C2'-C1'	6.82	123.20	113.12
3	B	1446	NAP	C2D-C1D-N1N	-6.55	102.77	113.86
3	C	1445	NAP	O4B-C1B-N9A	6.44	114.43	108.44
3	C	1445	NAP	O3-PN-O5D	-6.14	76.73	101.36
2	B	1447	CO8	C3'-C2'-C1'	6.03	122.02	113.12
2	D	1446	CO8	C3'-C2'-C1'	5.96	121.92	113.12
3	D	1445	NAP	O4D-C1D-N1N	-5.76	102.06	107.95
3	D	1445	NAP	O2X-P2B-O2B	5.42	122.69	107.09
3	D	1445	NAP	O3-PN-O5D	-5.26	80.30	101.36
2	C	1446	CO8	C2'-C1'-S1P	5.22	118.54	113.28
3	C	1445	NAP	O2B-P2B-O1X	5.17	121.23	106.79
2	A	1446	CO8	C2P-C3P-N4P	-5.01	101.17	112.50
3	D	1445	NAP	O4B-C1B-N9A	4.86	112.96	108.44
2	C	1446	CO8	N3A-C4A-N9A	4.74	134.00	125.43
3	A	1447	NAP	C3N-C7N-N7N	-4.65	112.48	117.77
3	D	1445	NAP	C3N-C7N-N7N	-4.61	112.52	117.77
3	C	1445	NAP	C2D-C1D-N1N	-4.56	106.14	113.86
3	A	1447	NAP	C2D-C1D-N1N	-4.40	106.40	113.86
2	D	1446	CO8	N3A-C4A-N9A	4.37	133.33	125.43
3	A	1447	NAP	C4D-O4D-C1D	-4.35	105.02	109.75
2	D	1446	CO8	C2'-C1'-S1P	4.30	117.61	113.28
2	B	1447	CO8	N3A-C4A-N9A	4.26	133.13	125.43
3	C	1445	NAP	C3N-C7N-N7N	-4.22	112.97	117.77
3	B	1446	NAP	N3A-C4A-N9A	4.11	132.86	125.43
3	A	1447	NAP	C2N-C3N-C4N	3.88	122.71	118.31
3	A	1447	NAP	O2B-P2B-O1X	-3.83	96.11	106.79
3	C	1445	NAP	N3A-C4A-N9A	3.77	132.24	125.43
2	A	1446	CO8	C3P-N4P-C5P	3.75	130.47	122.84
2	A	1446	CO8	N3A-C4A-N9A	3.74	132.19	125.43
2	C	1446	CO8	C3'-C2'-C1'	3.72	118.61	113.12
3	D	1445	NAP	N3A-C4A-N9A	3.71	132.13	125.43
3	D	1445	NAP	C2N-C3N-C4N	3.68	122.48	118.31
2	D	1446	CO8	O1'-C1'-S1P	-3.65	119.00	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1445	NAP	O2X-P2B-O1X	3.61	122.23	110.44
3	A	1447	NAP	N3A-C4A-N9A	3.55	131.84	125.43
3	C	1445	NAP	O4B-C1B-C2B	-3.31	103.85	106.95
2	C	1446	CO8	O1'-C1'-S1P	-3.30	119.38	122.85
3	B	1446	NAP	C8A-N9A-C4A	3.30	109.42	106.90
3	A	1447	NAP	P2B-O2B-C2B	-3.25	115.11	121.96
2	D	1446	CO8	O4B-C1B-N9A	-3.15	105.51	108.44
2	C	1446	CO8	C5A-C4A-N3A	-3.15	118.85	125.70
2	B	1447	CO8	P3B-O3B-C3B	-3.14	115.34	121.96
2	C	1446	CO8	C4'-C3'-C2'	2.95	124.40	113.28
2	A	1446	CO8	P3B-O3B-C3B	-2.94	115.76	121.96
3	D	1445	NAP	C2D-C1D-N1N	-2.91	108.93	113.86
3	D	1445	NAP	C5B-C4B-C3B	-2.89	103.64	115.21
2	D	1446	CO8	C5A-C4A-N3A	-2.88	119.42	125.70
3	B	1446	NAP	O2X-P2B-O2B	-2.85	98.87	107.09
3	A	1447	NAP	O3-PN-O1N	-2.80	102.13	108.83
3	D	1445	NAP	C8A-N9A-C4A	2.73	108.99	106.90
3	C	1445	NAP	O2N-PN-O5D	2.72	119.44	108.19
3	A	1447	NAP	O3D-C3D-C4D	-2.70	103.14	111.08
2	B	1447	CO8	C5A-C4A-N3A	-2.68	119.87	125.70
2	A	1446	CO8	O4B-C1B-N9A	2.67	110.92	108.44
3	A	1447	NAP	C3N-C2N-N1N	-2.65	115.90	120.36
2	B	1447	CO8	CEP-CBP-CAP	2.62	113.36	108.82
2	A	1446	CO8	O8A-P3B-O7A	-2.60	101.94	110.44
3	B	1446	NAP	PN-O3-PA	-2.59	121.83	132.95
3	A	1447	NAP	O3X-P2B-O2X	2.58	117.67	107.61
3	A	1447	NAP	O4D-C1D-C2D	-2.58	102.82	106.77
2	D	1446	CO8	C4'-C3'-C2'	2.57	122.98	113.28
3	D	1445	NAP	C4D-O4D-C1D	-2.57	106.96	109.75
3	C	1445	NAP	O7N-C7N-C3N	2.56	122.46	119.58
3	B	1446	NAP	C4D-O4D-C1D	-2.52	107.01	109.75
3	D	1445	NAP	O4B-C4B-C5B	-2.50	100.43	109.36
2	C	1446	CO8	C2A-N3A-C4A	2.48	121.08	114.01
3	D	1445	NAP	O7N-C7N-N7N	2.48	126.18	122.59
3	B	1446	NAP	N6A-C6A-N1A	2.45	124.17	119.36
3	B	1446	NAP	C3N-C7N-N7N	-2.42	115.02	117.77
2	A	1446	CO8	C6P-C5P-N4P	2.41	120.88	116.50
2	D	1446	CO8	O5A-P2A-O3A	2.39	116.47	105.14
3	D	1445	NAP	C2A-N3A-C4A	2.38	120.77	114.01
3	B	1446	NAP	C2A-N1A-C6A	2.37	123.05	118.77
2	D	1446	CO8	P2A-O3A-P1A	-2.37	124.74	131.68
2	C	1446	CO8	O5A-P2A-O3A	2.31	116.10	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1445	NAP	C2A-N1A-C6A	2.31	122.94	118.77
2	C	1446	CO8	O9A-P3B-O3B	2.30	113.72	107.09
2	D	1446	CO8	C2A-N3A-C4A	2.28	120.50	114.01
2	B	1447	CO8	C6'-C5'-C4'	-2.26	102.36	114.61
3	C	1445	NAP	C5A-C4A-N3A	-2.26	120.79	125.70
2	D	1446	CO8	C4A-C5A-N7A	-2.23	107.61	109.52
3	A	1447	NAP	PN-O3-PA	-2.21	123.48	132.95
3	D	1445	NAP	O2N-PN-O5D	2.20	117.28	108.19
2	B	1447	CO8	C2A-N3A-C4A	2.20	120.27	114.01
3	D	1445	NAP	O5D-PN-O1N	2.17	117.81	108.61
3	A	1447	NAP	C5A-C4A-N3A	-2.15	121.01	125.70
3	C	1445	NAP	C1B-N9A-C4A	-2.15	122.92	126.64
2	A	1446	CO8	C5A-C4A-N3A	-2.15	121.02	125.70
2	D	1446	CO8	C7P-C6P-C5P	-2.15	108.59	112.25
2	D	1446	CO8	C2P-S1P-C1'	-2.14	94.81	101.90
2	B	1447	CO8	O5A-P2A-O3A	2.14	115.29	105.14
2	B	1447	CO8	C4'-C3'-C2'	2.14	121.33	113.28
2	C	1446	CO8	O1'-C1'-C2'	-2.13	122.08	123.95
3	C	1445	NAP	C3D-C2D-C1D	-2.13	97.58	100.91
3	A	1447	NAP	O7N-C7N-C3N	2.13	121.97	119.58
3	D	1445	NAP	C1B-N9A-C4A	-2.12	122.97	126.64
3	D	1445	NAP	C5A-C4A-N3A	-2.11	121.09	125.70
2	A	1446	CO8	C1B-N9A-C4A	-2.10	123.00	126.64
2	B	1447	CO8	CEP-CBP-CCP	-2.10	105.73	108.76
2	C	1446	CO8	C4A-C5A-N7A	-2.09	107.73	109.52
3	C	1445	NAP	O2X-P2B-O1X	2.09	117.27	110.44
2	B	1447	CO8	C4A-C5A-N7A	-2.08	107.74	109.52
2	A	1446	CO8	CDP-CBP-CAP	2.08	112.43	108.82
3	B	1446	NAP	O3X-P2B-O1X	2.08	117.23	110.44
2	A	1446	CO8	C7P-C6P-C5P	-2.07	108.72	112.25
3	D	1445	NAP	N7A-C8A-N9A	-2.06	108.55	114.36
2	A	1446	CO8	O5P-C5P-N4P	-2.05	118.86	122.94
2	D	1446	CO8	C2P-C3P-N4P	-2.05	107.88	112.50
3	A	1447	NAP	C1B-N9A-C4A	-2.04	123.11	126.64
3	A	1447	NAP	O2N-PN-O3	2.03	114.26	108.79
3	A	1447	NAP	O3X-P2B-O1X	2.02	117.06	110.44
3	A	1447	NAP	O7N-C7N-N7N	2.02	125.51	122.59
3	C	1445	NAP	C8A-N9A-C4A	2.01	108.43	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	A	445/447 (99%)	0.50	9 (2%) 62 63	14, 20, 36, 46	1 (0%)
1	B	445/447 (99%)	0.52	12 (2%) 52 53	13, 20, 37, 47	1 (0%)
1	C	444/447 (99%)	0.42	12 (2%) 52 53	13, 21, 38, 58	3 (0%)
1	D	444/447 (99%)	0.51	12 (2%) 52 53	15, 23, 41, 58	0
All	All	1778/1788 (99%)	0.48	45 (2%) 54 56	13, 21, 39, 58	5 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	GLY	4.8
1	C	273	ALA	4.1
1	D	282	ALA	4.0
1	D	275	LEU	3.7
1	B	275	LEU	3.6
1	D	53	GLY	3.5
1	D	76	TYR	3.4
1	C	80	TRP	3.4
1	C	274	GLU	3.2
1	B	290	GLU	3.0
1	C	87	ILE	2.9
1	B	286	ARG	2.8
1	D	40	GLY	2.8
1	C	278	THR	2.7
1	A	13	ALA	2.7
1	C	281	ILE	2.6
1	A	207	TYR	2.6
1	C	76	TYR	2.5
1	A	274	GLU	2.5
1	B	157	LEU	2.5
1	B	142	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	363	ALA	2.4
1	C	435	ARG	2.4
1	A	211	VAL	2.3
1	B	210	LEU	2.3
1	A	363	ALA	2.3
1	B	274	GLU	2.3
1	D	273	ALA	2.3
1	A	275	LEU	2.3
1	B	150	ALA	2.3
1	B	273	ALA	2.3
1	D	80	TRP	2.3
1	D	87	ILE	2.3
1	D	276	GLY	2.3
1	A	41	VAL	2.2
1	C	36	ASP	2.2
1	B	211	VAL	2.2
1	A	273	ALA	2.2
1	D	435	ARG	2.2
1	D	274	GLU	2.1
1	C	279	ASP	2.1
1	D	279	ASP	2.1
1	A	370	ALA	2.1
1	B	445	THR	2.0
1	C	283	ASP	2.0

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

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

## 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO8	C	1446	57/57	0.36	4.51	11,78,88,88	0
2	CO8	D	1446	57/57	0.28	3.22	7,50,68,68	0
2	CO8	A	1446	57/57	0.21	1.99	2,27,40,41	0
2	CO8	B	1447	57/57	0.23	1.97	6,31,46,46	0
3	NAP	C	1445	48/48	0.15	0.64	10,18,25,27	0
3	NAP	D	1445	48/48	0.13	-0.54	10,15,23,23	0
3	NAP	B	1446	48/48	0.10	-1.33	2,9,16,17	0
3	NAP	A	1447	48/48	0.10	-1.82	2,8,14,16	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.