



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:01 pm GMT

PDB ID : 4FC7  
Title : Studies on DCR shed new light on peroxisomal beta-oxidation: Crystal structure of the ternary complex of pDCR  
Authors : Hua, T.; Wu, D.; Wang, J.; Shaw, N.; Liu, Z.-J.  
Deposited on : 2012-05-24  
Resolution : 1.84 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

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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 : 1.7.2 (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

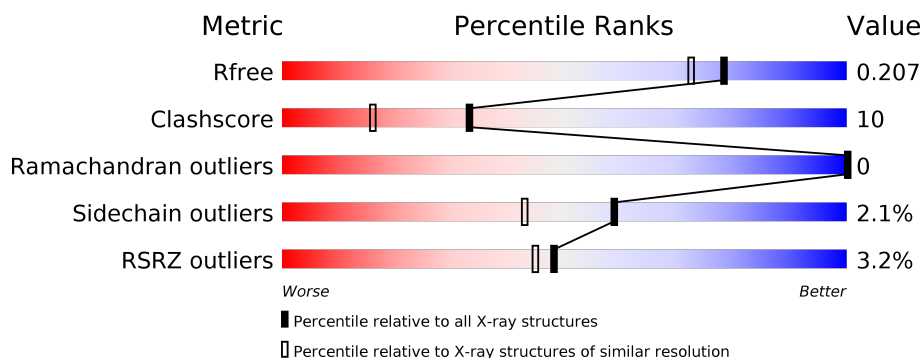
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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))
$R_{free}$	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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	A	277	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div></div> </div> <div></div> </div>
1	B	277	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div></div> </div> <div></div> </div>
1	C	277	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>16%</div> <div></div> </div> <div></div> </div>
1	D	277	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div></div> </div> <div></div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COA	C	402	-	-	-	X

## 2 Entry composition [i](#)

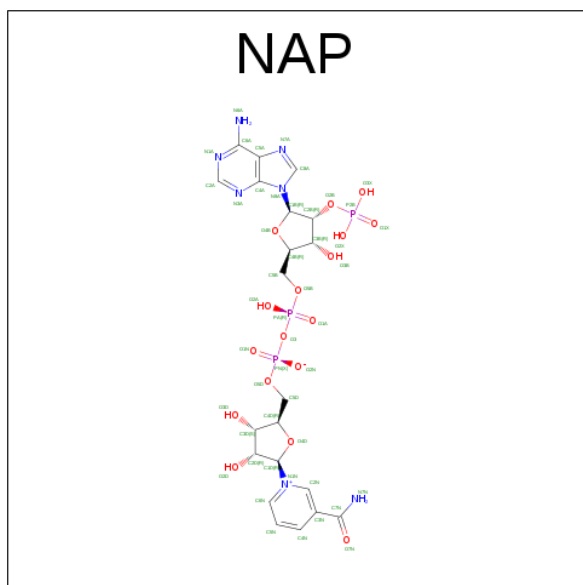
There are 4 unique types of molecules in this entry. The entry contains 9346 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peroxisomal 2,4-dienoyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	3	0
			2046	1296	371	366	13			
1	B	276	Total	C	N	O	S	0	1	0
			2051	1296	374	369	12			
1	C	276	Total	C	N	O	S	0	1	0
			2052	1297	374	369	12			
1	D	272	Total	C	N	O	S	0	1	0
			2021	1276	369	364	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



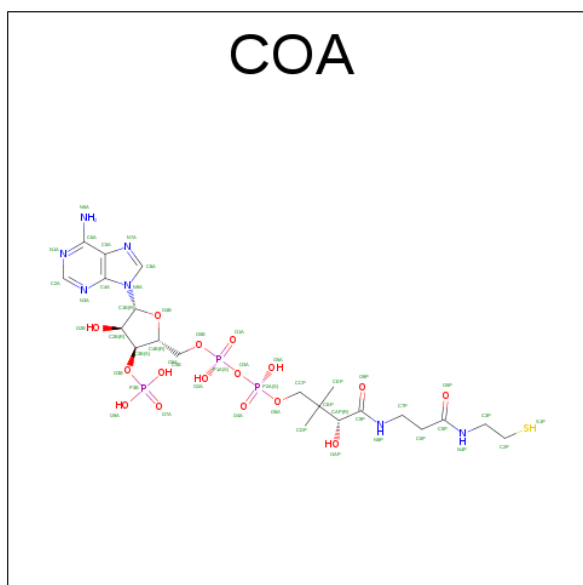
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total	O	0	0
			216	216		
4	B	176	Total	O	0	0
			176	176		
4	C	206	Total	O	0	0
			206	206		

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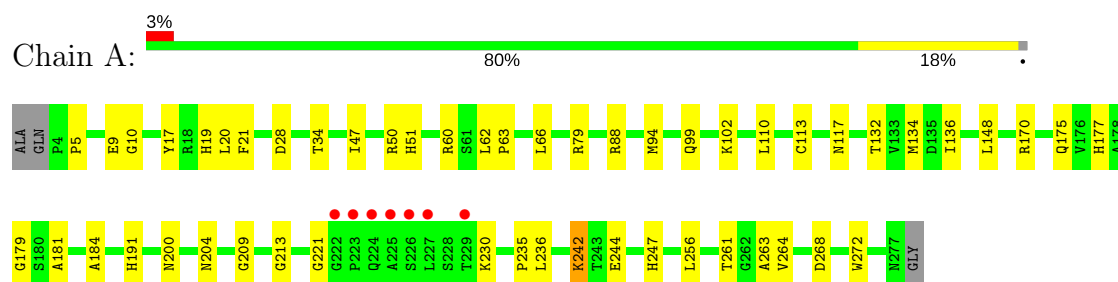
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	194	Total 194	O 194	0	0

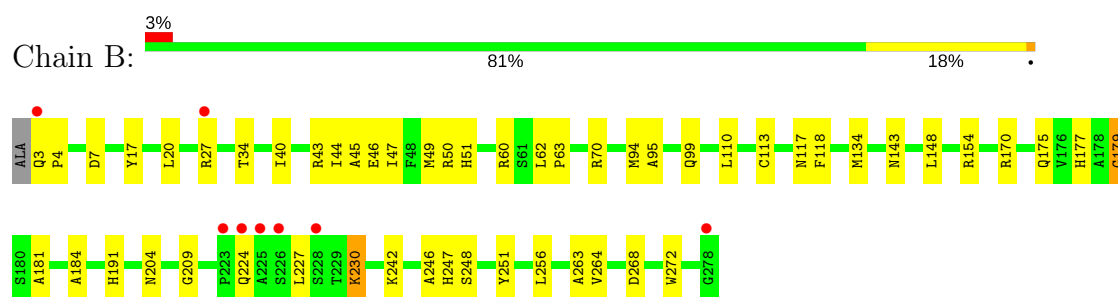
### 3 Residue-property plots

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.

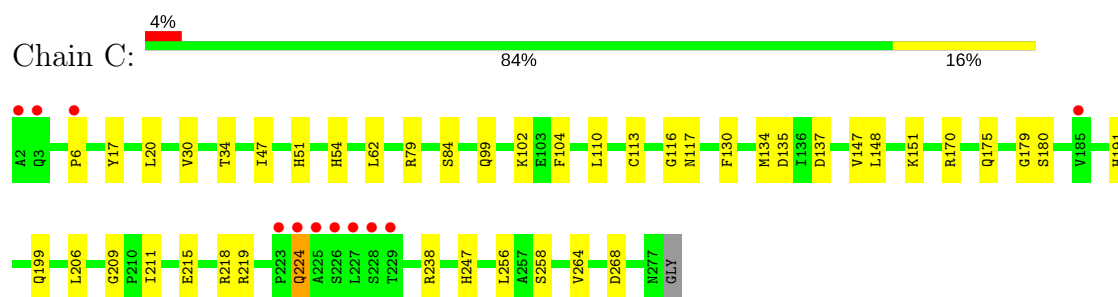
- Molecule 1: Peroxisomal 2,4-dienoyl-CoA reductase



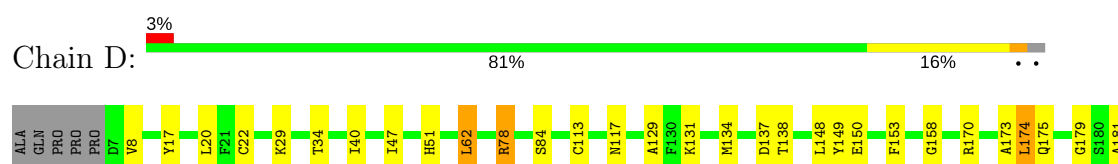
- Molecule 1: Peroxisomal 2,4-dienoyl-CoA reductase

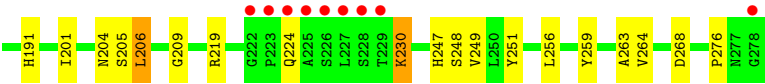


- Molecule 1: Peroxisomal 2,4-dienoyl-CoA reductase



- Molecule 1: Peroxisomal 2,4-dienoyl-CoA reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.10Å 94.50Å 130.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 1.84 38.92 – 1.84	Depositor EDS
% Data completeness (in resolution range)	97.9 (38.92-1.84) 97.9 (38.92-1.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.167 , 0.209 0.167 , 0.207	Depositor DCC
$R_{free}$ test set	4619 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: COA, 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	1.15	1/2098 (0.0%)	1.04	3/2850 (0.1%)
1	B	1.15	2/2097 (0.1%)	1.06	5/2849 (0.2%)
1	C	1.16	1/2098 (0.0%)	1.03	5/2851 (0.2%)
1	D	1.10	0/2064	1.04	6/2801 (0.2%)
All	All	1.14	4/8357 (0.0%)	1.04	19/11351 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	TRP	CD2-CE2	5.62	1.48	1.41
1	B	179	GLY	C-O	5.55	1.32	1.23
1	C	258	SER	CA-CB	5.19	1.60	1.52
1	B	272	TRP	CD2-CE2	5.02	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	C	206	LEU	CA-CB-CG	-5.91	101.71	115.30
1	D	62	LEU	CB-CG-CD2	-5.89	100.99	111.00
1	B	50	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	259	TYR	CD1-CE1-CZ	-5.68	114.69	119.80
1	C	219	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	206	LEU	CB-CG-CD2	-5.49	101.66	111.00
1	C	137	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	60	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	D	259	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	66	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	B	154	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	7	ASP	CB-CG-OD1	-5.22	113.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	79	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	154	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	135	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	236	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	D	259	TYR	OH-CZ-CE2	-5.04	106.50	120.10

There are no chirality outliers.

There are no planarity outliers.

## 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	A	2046	0	2087	49	0
1	B	2051	0	2081	48	0
1	C	2052	0	2083	35	0
1	D	2021	0	2052	46	0
2	A	48	0	25	2	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
3	A	48	0	32	0	0
3	B	48	0	32	0	0
3	C	48	0	32	1	0
3	D	48	0	32	2	0
4	A	216	0	0	17	0
4	B	176	0	0	14	0
4	C	206	0	0	7	0
4	D	194	0	0	13	0
All	All	9346	0	8531	168	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 10.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:HB3	4:B:674:HOH:O	1.39	1.23
1:B:70:ARG:HB3	4:B:676:HOH:O	1.45	1.13
1:D:138:THR:HB	4:D:691:HOH:O	1.45	1.11
1:A:200:ASN:HB3	4:A:555:HOH:O	1.58	1.03
1:A:132:THR:O	1:A:136[A]:ILE:HD13	1.59	1.03
1:D:206:LEU:HD23	1:D:249:VAL:HG22	1.44	0.98
1:D:206:LEU:HD23	1:D:249:VAL:CG2	2.01	0.91
1:D:230:LYS:HE2	4:D:629:HOH:O	1.71	0.90
1:A:134[A]:MET:HE1	1:A:177:HIS:O	1.73	0.87
1:A:88:ARG:HD3	1:A:136[A]:ILE:HD12	1.59	0.84
1:A:264:VAL:HG22	4:A:550:HOH:O	1.77	0.83
1:A:28:ASP:HA	4:A:716:HOH:O	1.80	0.82
1:B:117:ASN:HD21	1:B:175:GLN:HE22	1.26	0.82
1:C:110:LEU:HD22	1:C:148:LEU:HD12	1.60	0.81
1:B:94:MET:HE3	4:B:644:HOH:O	1.81	0.81
1:B:264:VAL:CG2	4:B:559:HOH:O	2.28	0.79
1:C:102:LYS:HE2	4:C:654:HOH:O	1.82	0.79
1:C:264:VAL:CG2	4:C:554:HOH:O	2.29	0.79
1:D:206:LEU:CD2	1:D:249:VAL:HG22	2.13	0.79
1:D:206:LEU:CD2	1:D:249:VAL:CG2	2.62	0.78
1:A:19:HIS:HD2	4:A:578:HOH:O	1.68	0.77
1:A:264:VAL:CG2	4:A:550:HOH:O	2.33	0.76
1:A:88:ARG:HD3	1:A:136[A]:ILE:CD1	2.17	0.75
1:C:117:ASN:HD21	1:C:175:GLN:HE22	1.35	0.75
1:B:47:ILE:O	1:B:51:HIS:HD2	1.69	0.74
1:C:47:ILE:O	1:C:51:HIS:HD2	1.72	0.73
1:A:88:ARG:NH2	1:A:136[A]:ILE:HD11	2.03	0.73
1:D:47:ILE:O	1:D:51:HIS:HD2	1.71	0.73
1:B:264:VAL:HG22	4:B:559:HOH:O	1.89	0.72
1:B:134[B]:MET:HE1	1:B:181:ALA:N	2.04	0.71
1:A:177:HIS:H	1:A:177:HIS:CD2	2.10	0.70
1:B:40:ILE:HD13	1:B:242:LYS:HG2	1.74	0.69
3:D:402:COA:H21	4:D:665:HOH:O	1.91	0.69
1:A:213:GLY:O	1:A:242:LYS:HE3	1.93	0.68
1:C:264:VAL:HG22	4:C:554:HOH:O	1.92	0.67
1:B:44:ILE:HD12	1:B:246:ALA:HA	1.77	0.67
1:C:17:TYR:OH	1:C:247:HIS:HE1	1.78	0.67
1:B:70:ARG:CB	4:B:676:HOH:O	2.21	0.67
1:D:40:ILE:HG23	4:D:690:HOH:O	1.95	0.67
1:D:17:TYR:OH	1:D:247:HIS:HE1	1.77	0.66
1:A:34:THR:O	1:A:113[B]:CYS:HB2	1.96	0.66
1:D:34:THR:O	1:D:113:CYS:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134[A]:MET:CE	1:A:181:ALA:HB2	2.26	0.65
1:A:117:ASN:HD21	1:A:175:GLN:HE22	1.44	0.65
1:A:17:TYR:OH	1:A:247:HIS:HE1	1.79	0.64
1:B:204:ASN:HD22	1:B:263:ALA:H	1.45	0.64
1:D:230:LYS:CE	4:D:629:HOH:O	2.38	0.64
1:A:47:ILE:O	1:A:51:HIS:HD2	1.83	0.61
1:B:256:LEU:HD21	1:D:20:LEU:HB2	1.81	0.61
1:D:206:LEU:CD2	1:D:249:VAL:HG23	2.29	0.61
1:C:134[A]:MET:HE3	1:C:180:SER:HB2	1.82	0.60
1:D:173:ALA:O	1:D:174:LEU:HB2	2.01	0.60
1:A:256:LEU:HD21	1:C:20:LEU:HB2	1.83	0.60
1:A:134[A]:MET:CE	1:A:177:HIS:O	2.49	0.60
1:D:204:ASN:HD22	1:D:263:ALA:H	1.49	0.60
1:C:224:GLN:HA	1:C:224:GLN:HE21	1.67	0.60
1:C:54:HIS:HE1	4:C:537:HOH:O	1.85	0.60
1:B:17:TYR:OH	1:B:247:HIS:HE1	1.85	0.59
1:B:27:ARG:HD2	4:B:628:HOH:O	2.02	0.59
1:B:44:ILE:CD1	1:B:246:ALA:HA	2.32	0.58
1:B:177:HIS:CD2	1:B:177:HIS:H	2.21	0.58
1:D:29:LYS:HE2	4:D:643:HOH:O	2.04	0.57
1:A:17:TYR:OH	1:A:247:HIS:CE1	2.57	0.57
1:D:51:HIS:HE1	4:D:513:HOH:O	1.87	0.57
1:B:110:LEU:HB2	1:B:148:LEU:HD13	1.87	0.56
1:C:110:LEU:HB2	1:C:148:LEU:CD1	2.35	0.56
1:D:175:GLN:NE2	4:D:592:HOH:O	2.37	0.56
1:B:204:ASN:ND2	1:B:263:ALA:H	2.02	0.56
1:D:117:ASN:HD21	1:D:175:GLN:HE22	1.53	0.56
1:D:205:SER:HB2	1:D:264:VAL:HG22	1.87	0.56
1:D:78:ARG:HG2	1:D:78:ARG:HH11	1.70	0.56
1:B:40:ILE:CD1	1:B:242:LYS:HG2	2.36	0.56
1:C:191:HIS:NE2	1:D:179:GLY:HA3	2.20	0.55
1:C:54:HIS:HD2	1:C:79:ARG:H	1.55	0.55
1:B:3:GLN:N	4:B:543:HOH:O	2.39	0.54
1:A:136[B]:ILE:HD11	4:A:715:HOH:O	2.06	0.54
1:C:264:VAL:HG23	4:C:554:HOH:O	2.01	0.54
1:D:134[B]:MET:HE2	1:D:181:ALA:HB2	1.90	0.54
1:C:209:GLY:O	1:C:211:ILE:HG12	2.08	0.53
1:B:95:ALA:O	1:B:99:GLN:HG3	2.08	0.53
1:B:117:ASN:ND2	1:B:175:GLN:HE22	2.03	0.53
1:B:134[B]:MET:HE2	1:B:181:ALA:HB2	1.91	0.53
1:A:191:HIS:NE2	1:B:179:GLY:HA3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LEU:HD23	1:D:249:VAL:HG23	1.90	0.53
1:D:276:PRO:HD3	4:D:667:HOH:O	2.08	0.53
1:D:78:ARG:HH11	1:D:78:ARG:CA	2.22	0.53
1:A:134[A]:MET:HE2	1:A:181:ALA:HB2	1.91	0.52
1:B:94:MET:CE	4:B:644:HOH:O	2.48	0.52
1:C:17:TYR:OH	1:C:247:HIS:CE1	2.62	0.52
1:D:62:LEU:HB2	1:D:84:SER:HB2	1.92	0.52
1:D:204:ASN:ND2	1:D:263:ALA:H	2.07	0.51
1:A:221:GLY:HA3	4:A:584:HOH:O	2.10	0.51
1:D:78:ARG:HG2	1:D:78:ARG:NH1	2.26	0.51
1:B:148:LEU:HD23	4:B:675:HOH:O	2.11	0.50
1:A:21:PHE:HB2	1:A:51:HIS:CE1	2.46	0.50
1:C:102:LYS:HD2	4:C:639:HOH:O	2.11	0.50
1:B:62:LEU:HB3	1:B:63:PRO:HD3	1.92	0.50
1:C:134[A]:MET:CE	1:C:180:SER:HB2	2.42	0.50
1:C:6:PRO:HD2	4:C:611:HOH:O	2.12	0.50
1:D:209:GLY:HA3	1:D:268:ASP:HB2	1.94	0.49
1:B:248:SER:OG	1:D:251:TYR:OH	2.24	0.49
1:D:78:ARG:HA	1:D:78:ARG:HH11	1.75	0.49
1:A:19:HIS:HE1	1:A:50:ARG:O	1.95	0.49
1:A:110:LEU:HB2	1:A:148:LEU:HD13	1.94	0.49
1:A:94:MET:CE	4:A:560:HOH:O	2.61	0.48
2:A:401:NAP:H52A	4:A:709:HOH:O	2.12	0.48
1:A:204:ASN:HD21	1:A:261:THR:HA	1.78	0.48
1:D:22:CYS:HB2	4:D:692:HOH:O	2.14	0.48
1:D:134[B]:MET:CE	1:D:181:ALA:HB2	2.44	0.48
1:A:51:HIS:HE1	4:A:504:HOH:O	1.95	0.48
1:C:116:GLY:HA3	3:C:402:COA:H142	1.95	0.47
1:C:117:ASN:HD21	1:C:175:GLN:NE2	2.08	0.47
1:B:47:ILE:HG13	1:B:246:ALA:CB	2.45	0.47
1:C:209:GLY:HA3	1:C:268:ASP:HB2	1.96	0.47
4:B:518:HOH:O	1:D:247:HIS:HD2	1.96	0.47
1:D:78:ARG:HH11	1:D:78:ARG:CG	2.28	0.47
1:B:264:VAL:HG23	4:B:508:HOH:O	2.14	0.47
2:A:401:NAP:H52N	4:A:709:HOH:O	2.14	0.47
1:B:34:THR:O	1:B:113:CYS:HB3	2.15	0.46
1:A:204:ASN:HD22	1:A:263:ALA:H	1.62	0.46
1:A:179:GLY:HA3	1:B:191:HIS:NE2	2.30	0.46
1:B:170:ARG:HD2	1:C:170:ARG:HD2	1.97	0.46
1:B:143:ASN:CB	4:B:674:HOH:O	2.23	0.45
1:C:179:GLY:HA3	1:D:191:HIS:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:HB2	1:C:148:LEU:HD12	1.97	0.45
1:B:43:ARG:O	1:B:47:ILE:HG12	2.17	0.45
1:B:247:HIS:HD2	4:D:557:HOH:O	2.00	0.44
1:B:230:LYS:HE3	1:B:230:LYS:HB3	1.70	0.44
1:D:137:ASP:HB2	1:D:181:ALA:HB1	1.99	0.44
1:C:62:LEU:HB2	1:C:84:SER:HB2	1.99	0.43
1:A:209:GLY:CA	1:A:268:ASP:HB2	2.48	0.43
1:A:62:LEU:N	1:A:63:PRO:CD	2.82	0.43
1:A:60:ARG:NH1	4:A:715:HOH:O	2.51	0.43
1:A:184:ALA:HB2	1:B:184:ALA:HB2	2.00	0.43
1:A:209:GLY:HA3	1:A:268:ASP:HB2	2.01	0.43
1:D:17:TYR:OH	1:D:247:HIS:CE1	2.64	0.42
1:A:204:ASN:HD21	1:A:261:THR:CA	2.32	0.42
1:C:34:THR:O	1:C:113:CYS:HB3	2.18	0.42
1:A:28:ASP:CA	4:A:716:HOH:O	2.53	0.42
1:B:118:PHE:O	1:B:177:HIS:HE1	2.03	0.42
1:D:173:ALA:HA	4:D:524:HOH:O	2.19	0.42
1:B:251:TYR:HH	1:D:248:SER:HG	1.65	0.42
1:B:20:LEU:HA	4:D:692:HOH:O	2.18	0.42
1:C:147:VAL:O	1:C:151:LYS:HG2	2.20	0.42
1:A:5:PRO:HD2	1:A:244:GLU:HG2	2.01	0.41
1:B:3:GLN:HA	1:B:4:PRO:HD3	1.96	0.41
1:C:130:PHE:CZ	1:C:134[A]:MET:HE3	2.55	0.41
1:C:30:VAL:HG21	1:C:104:PHE:HB3	2.02	0.41
1:A:9:GLU:HG2	1:A:10:GLY:N	2.35	0.41
1:A:88:ARG:HD3	1:A:136[A]:ILE:HD11	2.00	0.41
1:B:20:LEU:HB2	1:D:256:LEU:HD21	2.02	0.41
1:B:264:VAL:HG23	4:B:559:HOH:O	2.11	0.41
1:A:94:MET:HE3	4:A:560:HOH:O	2.20	0.41
1:B:43:ARG:NH1	1:B:46:GLU:OE1	2.53	0.41
1:D:149:TYR:HA	1:D:153:PHE:HB2	2.03	0.41
1:A:99:GLN:NE2	4:A:714:HOH:O	2.50	0.41
4:A:516:HOH:O	1:C:247:HIS:HD2	2.04	0.41
1:D:158:GLY:O	1:D:201:ILE:HA	2.21	0.41
1:B:45:ALA:O	1:B:49:MET:HG3	2.21	0.41
1:C:215:GLU:HA	1:C:218:ARG:HE	1.86	0.41
1:B:209:GLY:HA3	1:B:268:ASP:HB2	2.03	0.41
1:C:148:LEU:HA	1:C:148:LEU:HD23	1.74	0.40
1:D:129:ALA:HB2	3:D:402:COA:H1B	2.02	0.40
1:A:20:LEU:HB2	1:C:256:LEU:HD21	2.03	0.40
1:A:94:MET:HE2	4:A:560:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HD2	1:D:170:ARG:HD2	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	275/277 (99%)	270 (98%)	5 (2%)	0	100	100
1	B	275/277 (99%)	270 (98%)	5 (2%)	0	100	100
1	C	275/277 (99%)	271 (98%)	4 (2%)	0	100	100
1	D	271/277 (98%)	266 (98%)	5 (2%)	0	100	100
All	All	1096/1108 (99%)	1077 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	214/212 (101%)	210 (98%)	4 (2%)	62	47
1	B	213/212 (100%)	210 (99%)	3 (1%)	71	60
1	C	213/212 (100%)	210 (99%)	3 (1%)	71	60
1	D	209/212 (99%)	201 (96%)	8 (4%)	38	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	849/848 (100%)	831 (98%)	18 (2%)	59 43

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	230	LYS
1	A	235	PRO
1	A	242	LYS
1	B	224	GLN
1	B	227	LEU
1	B	230	LYS
1	C	99	GLN
1	C	199	GLN
1	C	224	GLN
1	D	8	VAL
1	D	78	ARG
1	D	131	LYS
1	D	148	LEU
1	D	150	GLU
1	D	174	LEU
1	D	224	GLN
1	D	230	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	51	HIS
1	A	99	GLN
1	A	112	ASN
1	A	175	GLN
1	A	177	HIS
1	A	204	ASN
1	A	247	HIS
1	B	19	HIS
1	B	51	HIS
1	B	112	ASN
1	B	175	GLN
1	B	177	HIS
1	B	204	ASN

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Mol	Chain	Res	Type
1	B	247	HIS
1	C	51	HIS
1	C	54	HIS
1	C	112	ASN
1	C	175	GLN
1	C	224	GLN
1	C	247	HIS
1	D	51	HIS
1	D	112	ASN
1	D	175	GLN
1	D	204	ASN
1	D	224	GLN
1	D	247	HIS

### 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](#)

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	NAP	A	401	-	44,52,52	1.38	6 (13%)	51,80,80	1.81	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	COA	A	402	-	43,50,50	1.15	3 (6%)	48,75,75	2.29	15 (31%)
2	NAP	B	401	-	44,52,52	1.25	5 (11%)	51,80,80	1.89	9 (17%)
3	COA	B	402	-	43,50,50	1.04	3 (6%)	48,75,75	2.19	11 (22%)
2	NAP	C	401	-	44,52,52	1.38	6 (13%)	51,80,80	1.55	5 (9%)
3	COA	C	402	-	43,50,50	1.11	2 (4%)	48,75,75	1.83	9 (18%)
2	NAP	D	401	-	44,52,52	1.35	6 (13%)	51,80,80	1.29	7 (13%)
3	COA	D	402	-	43,50,50	1.25	4 (9%)	48,75,75	1.47	4 (8%)

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	NAP	A	401	-	-	0/27/67/67	0/5/5/5
3	COA	A	402	-	-	0/44/64/64	0/3/3/3
2	NAP	B	401	-	-	0/27/67/67	0/5/5/5
3	COA	B	402	-	-	0/44/64/64	0/3/3/3
2	NAP	C	401	-	-	0/27/67/67	0/5/5/5
3	COA	C	402	-	-	0/44/64/64	0/3/3/3
2	NAP	D	401	-	-	0/27/67/67	0/5/5/5
3	COA	D	402	-	-	0/44/64/64	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	C5A-N7A	-2.22	1.31	1.39
2	D	401	NAP	C4N-C3N	2.02	1.42	1.39
3	D	402	COA	O4B-C1B	2.05	1.44	1.41
2	D	401	NAP	O3B-C3B	2.07	1.47	1.43
2	B	401	NAP	C5D-C4D	2.17	1.58	1.51
3	B	402	COA	C2B-C1B	2.22	1.57	1.53
2	B	401	NAP	C7N-N7N	2.26	1.37	1.33
2	A	401	NAP	C2A-N1A	2.30	1.38	1.33
3	B	402	COA	C5A-C4A	2.36	1.45	1.40
2	D	401	NAP	C6N-C5N	2.41	1.43	1.38
3	D	402	COA	C4A-N3A	2.42	1.39	1.35
3	B	402	COA	P3B-O3B	2.45	1.63	1.59
2	B	401	NAP	C2A-N3A	2.55	1.36	1.32
2	A	401	NAP	O4B-C1B	2.61	1.44	1.41
3	A	402	COA	O4B-C1B	2.65	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	COA	P3B-O3B	2.67	1.64	1.59
2	C	401	NAP	O3B-C3B	2.67	1.49	1.43
2	A	401	NAP	C2A-N3A	2.69	1.36	1.32
2	D	401	NAP	O4D-C1D	2.71	1.45	1.41
2	D	401	NAP	C5A-C4A	2.74	1.46	1.40
3	C	402	COA	C5A-C4A	2.77	1.46	1.40
3	A	402	COA	P3B-O3B	2.80	1.64	1.59
2	C	401	NAP	C5A-C4A	2.85	1.46	1.40
2	C	401	NAP	O4D-C1D	2.86	1.45	1.41
2	C	401	NAP	C4A-N3A	2.92	1.39	1.35
2	C	401	NAP	C4N-C3N	3.08	1.44	1.39
3	A	402	COA	C5A-C4A	3.19	1.47	1.40
2	A	401	NAP	C5A-C4A	3.20	1.47	1.40
2	A	401	NAP	P2B-O2B	3.33	1.65	1.59
3	C	402	COA	C2A-N3A	3.44	1.37	1.32
2	B	401	NAP	P2B-O2B	3.51	1.65	1.59
3	D	402	COA	C5A-C4A	3.62	1.48	1.40
2	C	401	NAP	P2B-O2B	4.14	1.66	1.59
2	A	401	NAP	C4N-C3N	4.27	1.46	1.39
2	D	401	NAP	P2B-O2B	4.94	1.68	1.59

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	N3A-C2A-N1A	-9.22	120.82	128.86
2	B	401	NAP	N3A-C2A-N1A	-8.61	121.36	128.86
3	B	402	COA	N3A-C2A-N1A	-8.29	121.64	128.86
2	A	401	NAP	N3A-C2A-N1A	-8.06	121.84	128.86
3	C	402	COA	N3A-C2A-N1A	-7.04	122.73	128.86
3	B	402	COA	CEP-CBP-CCP	-7.03	98.05	108.37
2	C	401	NAP	N3A-C2A-N1A	-6.34	123.33	128.86
3	A	402	COA	CEP-CBP-CCP	-5.74	99.95	108.37
3	D	402	COA	CEP-CBP-CCP	-5.30	100.59	108.37
3	D	402	COA	N3A-C2A-N1A	-4.94	124.55	128.86
3	C	402	COA	CDP-CBP-CAP	-4.24	101.47	108.82
3	C	402	COA	C1B-N9A-C4A	-3.80	120.07	126.64
2	D	401	NAP	N3A-C2A-N1A	-3.36	125.94	128.86
3	B	402	COA	O6A-CCP-CBP	-3.32	105.21	110.55
2	B	401	NAP	C1B-N9A-C4A	-3.18	121.14	126.64
2	A	401	NAP	C5N-C4N-C3N	-3.18	116.61	120.35
3	A	402	COA	C4A-C5A-N7A	-3.17	106.35	109.41
3	A	402	COA	C3P-N4P-C5P	-3.12	116.86	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	COA	OAP-CAP-CBP	-3.08	103.00	110.25
2	B	401	NAP	C4B-O4B-C1B	-3.06	106.51	109.77
2	C	401	NAP	C3N-C2N-N1N	-3.04	117.37	120.43
2	B	401	NAP	O5B-C5B-C4B	-2.96	98.49	109.00
3	A	402	COA	O3B-P3B-O7A	-2.84	98.15	109.26
2	A	401	NAP	C4A-C5A-N7A	-2.73	106.78	109.41
3	B	402	COA	O5B-P1A-O1A	-2.51	99.14	109.25
3	C	402	COA	OAP-CAP-CBP	-2.36	104.69	110.25
3	B	402	COA	O6A-P2A-O4A	-2.34	99.82	109.25
3	A	402	COA	C1B-N9A-C4A	-2.33	122.60	126.64
2	A	401	NAP	O7N-C7N-C3N	-2.32	116.91	119.62
3	C	402	COA	O6A-CCP-CBP	-2.26	106.91	110.55
2	A	401	NAP	C1B-N9A-C4A	-2.25	122.75	126.64
2	D	401	NAP	O3D-C3D-C2D	-2.24	104.66	111.83
2	C	401	NAP	O5B-C5B-C4B	-2.17	101.30	109.00
3	B	402	COA	O3B-C3B-C4B	-2.14	102.02	110.04
3	A	402	COA	C2B-C3B-C4B	-2.06	99.54	103.23
3	A	402	COA	CDP-CBP-CAP	-2.05	105.27	108.82
2	D	401	NAP	C4B-O4B-C1B	-2.04	107.59	109.77
3	D	402	COA	C5B-C4B-C3B	-2.04	107.39	114.30
3	C	402	COA	O2A-P1A-O1A	2.01	122.69	112.28
2	C	401	NAP	C3N-C7N-N7N	2.10	120.17	117.77
2	D	401	NAP	C2A-N1A-C6A	2.11	122.46	118.77
3	A	402	COA	O6A-CCP-CBP	2.12	113.96	110.55
3	A	402	COA	O4B-C4B-C3B	2.14	109.53	104.81
2	A	401	NAP	C2A-N1A-C6A	2.22	122.66	118.77
2	B	401	NAP	C2A-N1A-C6A	2.26	122.72	118.77
2	B	401	NAP	O2X-P2B-O1X	2.28	119.42	110.50
3	B	402	COA	O9A-P3B-O7A	2.30	119.48	110.50
2	C	401	NAP	O2X-P2B-O1X	2.30	119.49	110.50
3	B	402	COA	CDP-CBP-CCP	2.30	111.74	108.37
3	C	402	COA	O9A-P3B-O7A	2.32	119.56	110.50
3	A	402	COA	O5P-C5P-C6P	2.32	126.36	122.01
2	D	401	NAP	O2A-PA-O1A	2.39	124.65	112.28
3	A	402	COA	C6P-C7P-N8P	2.39	116.82	111.87
2	B	401	NAP	O3X-P2B-O1X	2.45	120.10	110.50
2	A	401	NAP	C4D-O4D-C1D	2.52	112.45	109.77
2	A	401	NAP	N6A-C6A-N1A	2.56	123.84	118.77
2	D	401	NAP	O3X-P2B-O2X	2.57	117.99	107.61
3	A	402	COA	C2A-N1A-C6A	2.57	123.27	118.77
3	C	402	COA	CEP-CBP-CAP	2.78	113.64	108.82
3	D	402	COA	O2A-P1A-O1A	2.82	126.85	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	O2X-P2B-O1X	2.82	121.52	110.50
2	D	401	NAP	N6A-C6A-N1A	2.96	124.63	118.77
3	C	402	COA	N6A-C6A-N1A	3.01	124.72	118.77
2	B	401	NAP	N6A-C6A-N1A	3.01	124.74	118.77
3	B	402	COA	O2A-P1A-O1A	3.16	128.62	112.28
3	B	402	COA	C2A-N1A-C6A	3.23	124.42	118.77
3	B	402	COA	O5A-P2A-O6A	3.36	123.99	108.14
2	A	401	NAP	C2N-C3N-C4N	3.40	122.14	118.26
2	B	401	NAP	O2N-PN-O1N	3.55	130.68	112.28
3	A	402	COA	CDP-CBP-CCP	3.65	113.73	108.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	2	0
3	C	402	COA	1	0
3	D	402	COA	2	0

## 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	A	274/277 (98%)	-0.14	7 (2%) 56 53	6, 14, 30, 53	0
1	B	276/277 (99%)	-0.13	8 (2%) 52 49	8, 17, 31, 56	0
1	C	276/277 (99%)	-0.01	11 (3%) 39 35	6, 15, 33, 63	0
1	D	272/277 (98%)	-0.14	9 (3%) 47 44	7, 16, 33, 55	0
All	All	1098/1108 (99%)	-0.10	35 (3%) 48 45	6, 15, 32, 63	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	6.0
1	D	225	ALA	5.1
1	C	224	GLN	4.9
1	C	223	PRO	4.8
1	A	224	GLN	4.8
1	D	223	PRO	4.8
1	C	2	ALA	4.5
1	A	225	ALA	4.5
1	C	225	ALA	4.1
1	B	224	GLN	3.7
1	D	226	SER	3.6
1	B	223	PRO	3.5
1	D	222	GLY	3.4
1	A	222	GLY	3.4
1	D	227	LEU	3.4
1	A	223	PRO	3.3
1	A	226	SER	3.1
1	B	226	SER	3.1
1	D	224	GLN	3.1
1	D	228	SER	3.0
1	A	227	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	226	SER	2.7
1	D	278	GLY	2.7
1	C	229	THR	2.7
1	C	227	LEU	2.6
1	D	229	THR	2.6
1	C	6	PRO	2.5
1	A	229	THR	2.4
1	B	3	GLN	2.4
1	C	3	GLN	2.2
1	B	278	GLY	2.2
1	B	228	SER	2.1
1	C	228	SER	2.1
1	C	185	VAL	2.1
1	B	27	ARG	2.1

## 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](#)

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(Å <sup>2</sup> )	Q<0.9
3	COA	C	402	48/48	0.93	0.17	2.05	21,25,30,57	0
3	COA	D	402	48/48	0.93	0.14	1.55	21,26,34,40	0
3	COA	A	402	48/48	0.93	0.14	1.46	19,25,33,48	0
3	COA	B	402	48/48	0.95	0.09	-0.18	12,20,27,40	0
2	NAP	C	401	48/48	0.97	0.06	-0.94	13,17,20,21	0
2	NAP	D	401	48/48	0.98	0.07	-0.94	11,17,20,20	0
2	NAP	B	401	48/48	0.98	0.07	-0.99	11,14,18,20	0
2	NAP	A	401	48/48	0.98	0.06	-1.05	11,17,20,21	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.