



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:59 am 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 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

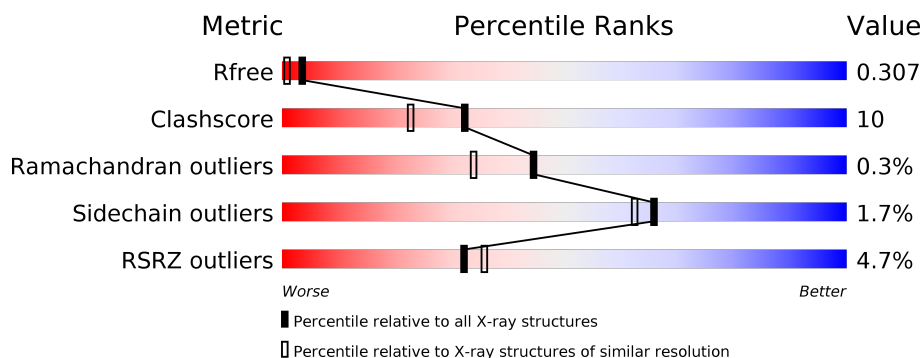
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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. 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	447	<div> <div>3%</div> <div>82%</div> <div>17%</div> </div>
1	B	447	<div> <div>4%</div> <div>82%</div> <div>17%</div> </div>
1	C	447	<div> <div>4%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
1	D	447	<div> <div>7%</div> <div>77%</div> <div>21%</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
2	CO8	A	1446	-	-	-	X
2	CO8	B	1447	-	-	-	X
2	CO8	C	1446	-	-	-	X
2	CO8	D	1446	-	-	-	X

## 2 Entry composition [i](#)

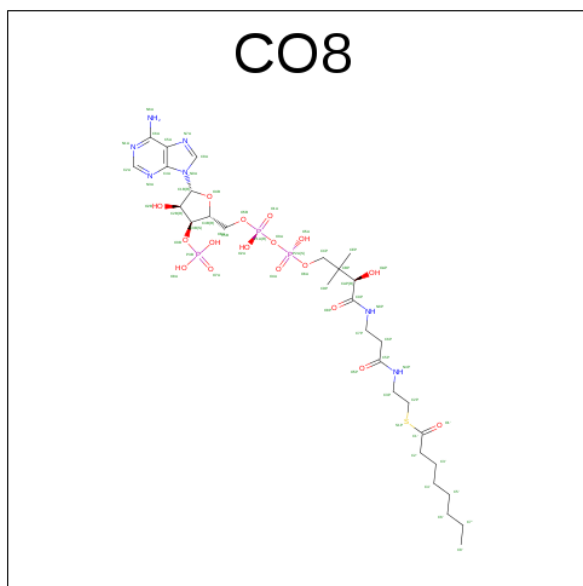
There are 4 unique types of molecules in this entry. The entry contains 15766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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:  $C_{29}H_{50}N_7O_{17}P_3S$ ).



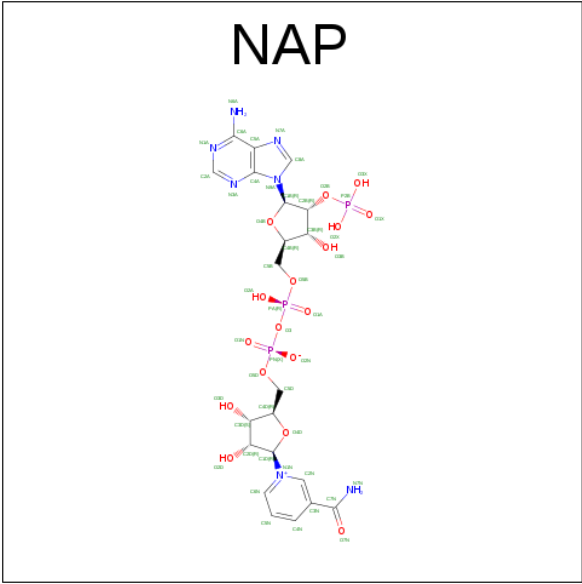
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			57	29	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			57	29	7	17	3 1		

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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-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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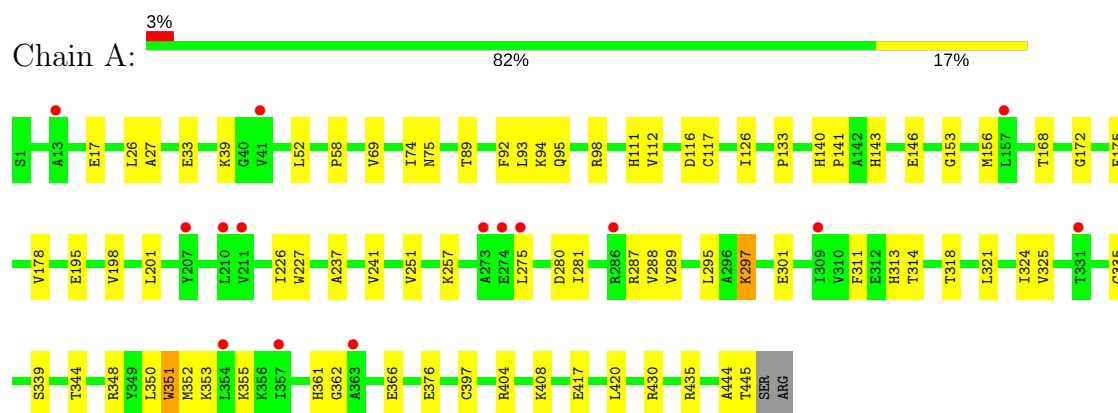
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	431	Total 431	O 431	0	0

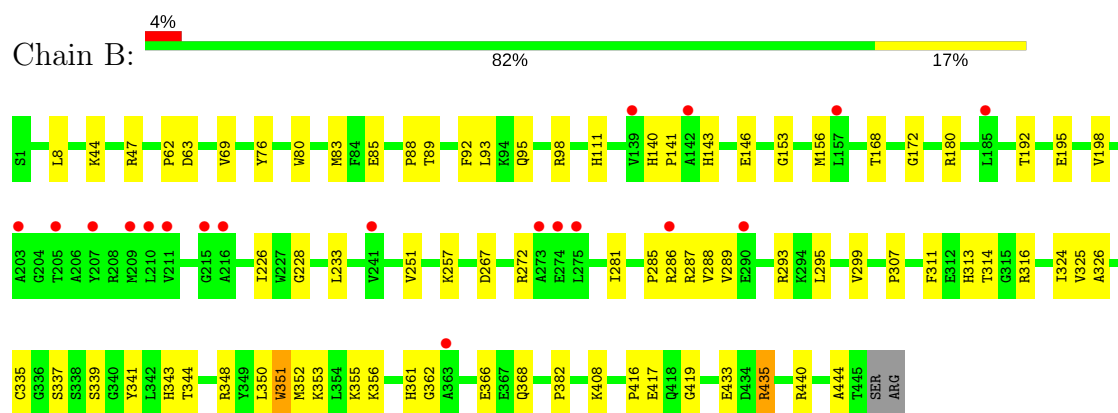
### 3 Residue-property plots [i](#)

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.

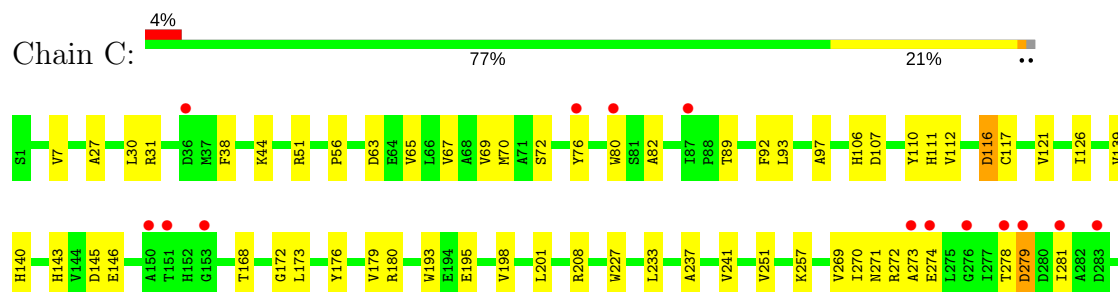
#### • Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

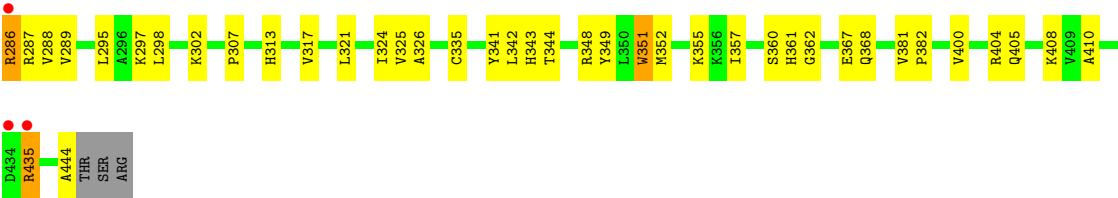


#### • Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE

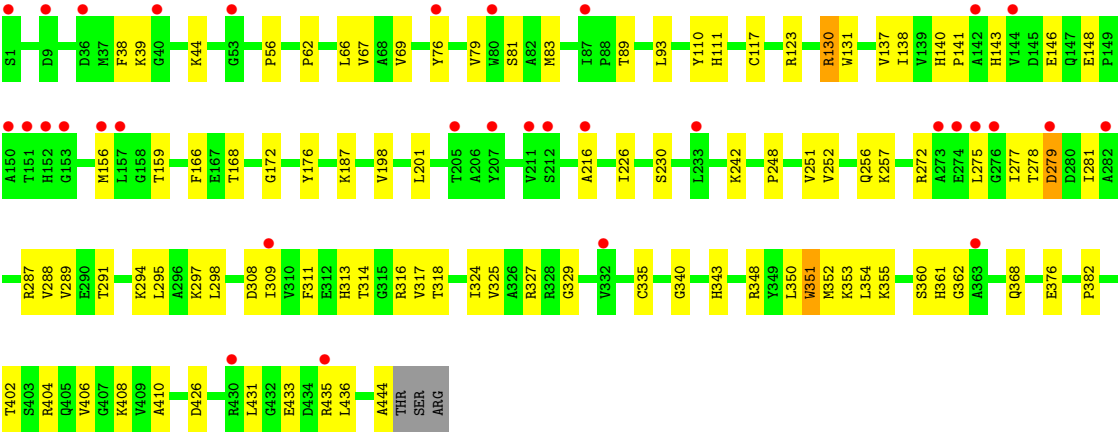
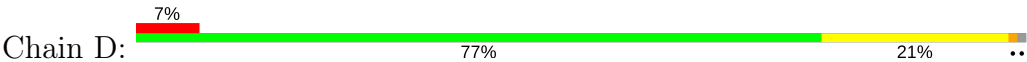


#### • Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE





● Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE





## 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 0.262 , 0.307	Depositor DCC
$R_{free}$ test set	7035 reflections (5.00%)	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> )	0.37 , 15.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.91	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.

<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

### 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 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	3375	0	3369	59	0
1	B	3371	0	3368	70	0
1	C	3360	0	3349	80	0
1	D	3348	0	3335	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	57	0	46	2	0
2	B	57	0	46	4	0
2	C	57	0	46	5	0
2	D	57	0	46	5	0
3	A	48	0	25	7	0
3	B	48	0	25	9	0
3	C	48	0	25	6	0
3	D	48	0	25	5	0
4	A	522	0	0	6	0
4	B	482	0	0	8	0
4	C	457	0	0	6	0
4	D	431	0	0	9	0
All	All	15766	0	13705	276	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 (276) 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:D:79:VAL:HG12	1:D:83:MET:HE2	1.28	1.07
1:D:79:VAL:HG12	1:D:83:MET:CE	1.91	0.99
1:B:228:GLY:H	1:B:272[B]:ARG:HH22	1.11	0.97
1:C:362:GLY:H	3:C:1445:NAP:H72N	1.13	0.94
1:D:362:GLY:H	3:D:1445:NAP:H72N	1.06	0.94
1:A:362:GLY:H	3:A:1447:NAP:H72N	1.03	0.93
1:B:362:GLY:H	3:B:1446:NAP:H72N	0.89	0.88
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
1:B:295:LEU:HD23	1:B:325:VAL:HG11	1.57	0.84
1:B:267:ASP:HB3	4:B:2307:HOH:O	1.77	0.84
1:C:233:LEU:HD21	1:C:335:CYS:SG	2.22	0.79
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:D:281:ILE:HG13	1:D:287:ARG:HG2	1.66	0.76
1:C:297:LYS:HD3	4:C:2321:HOH:O	1.86	0.74
1:A:275:LEU:HD11	1:A:295:LEU:HD13	1.74	0.69
1:A:17:GLU:HG2	1:A:133:PRO:HG2	1.72	0.69
1:C:362:GLY:N	3:C:1445:NAP:H72N	1.89	0.67
1:C:63:ASP:OD2	4:C:2120:HOH:O	2.12	0.67
1:D:148:GLU:OE2	1:D:159:THR:HB	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:HD23	1:C:325:VAL:HG11	1.75	0.67
1:D:376:GLU:OE1	4:D:2347:HOH:O	2.14	0.66
1:B:286:ARG:HH12	1:B:293[A]:ARG:NH2	1.94	0.65
1:A:362:GLY:N	3:A:1447:NAP:H72N	1.87	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:B:286:ARG:HH12	1:B:293[A]:ARG:HH22	1.46	0.63
2:B:1447:CO8:O7A	1:C:286:ARG:NH2	2.29	0.63
1:A:280:ASP:OD1	1:A:287[A]:ARG:NH2	2.32	0.63
1:C:278:THR:O	1:C:281:ILE:HG22	1.98	0.63
1:B:80:TRP:CE3	1:B:83:MET:CE	2.83	0.62
1:B:95:GLN:HG2	1:B:98:ARG:HH12	1.64	0.62
1:D:79:VAL:CG1	1:D:83:MET:CE	2.73	0.62
1:D:256:GLN:HG2	4:D:2262:HOH:O	1.98	0.62
1:D:278:THR:O	1:D:281:ILE:HG22	2.00	0.61
1:D:279:ASP:HA	1:D:317:VAL:HG12	1.82	0.61
1:A:289:VAL:HA	1:A:324:ILE:HD13	1.82	0.61
1:B:281:ILE:HG13	1:B:287:ARG:HG2	1.81	0.61
1:B:80:TRP:CE3	1:B:83:MET:HE3	2.36	0.61
1:C:289:VAL:HA	1:C:324:ILE:HD13	1.84	0.60
1:B:348:ARG:O	1:B:352:MET:HB2	2.01	0.60
1:B:80:TRP:HE3	1:B:83:MET:HE3	1.68	0.59
2:B:1447:CO8:P3B	1:C:286:ARG:HH22	2.26	0.59
1:D:317:VAL:HG23	1:D:318:THR:HG23	1.84	0.58
1:B:63:ASP:OD2	4:B:2102:HOH:O	2.16	0.58
1:B:295:LEU:CD2	1:B:325:VAL:HG11	2.30	0.57
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:B:228:GLY:H	1:B:272[B]:ARG:NH2	1.93	0.57
1:A:95:GLN:HG2	1:A:98:ARG:NH1	2.20	0.56
1:A:335:CYS:O	3:A:1447:NAP:H2N	2.06	0.56
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:D:295:LEU:HG	1:D:325:VAL:HG11	1.89	0.55
1:C:335:CYS:O	3:C:1445:NAP:H2N	2.07	0.55
1:A:417:GLU:HG2	1:A:420:LEU:HD11	1.90	0.54
3:B:1446:NAP:H8A	3:B:1446:NAP:H3B	1.89	0.54
1:C:404:ARG:NH2	4:C:2092:HOH:O	2.40	0.54
1:C:198:VAL:O	1:C:408:LYS:HE2	2.07	0.54
1:D:348:ARG:O	1:D:352:MET:HB2	2.08	0.54
1:D:297:LYS:NZ	4:D:2297:HOH:O	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LEU:HD11	2:D:1446:CO8:H4'1	1.89	0.54
1:A:95:GLN:HG2	1:A:98:ARG:HH12	1.74	0.53
1:C:56:PRO:HD2	1:C:110:TYR:CZ	2.43	0.53
1:C:307:PRO:HD2	1:C:325:VAL:O	2.08	0.53
1:D:81:SER:HB2	1:D:89:THR:HG21	1.90	0.53
1:A:146[B]:GLU:HB2	1:B:146:GLU:HB3	1.91	0.53
1:C:348:ARG:O	1:C:352:MET:HB2	2.08	0.53
1:D:198:VAL:O	1:D:408:LYS:HE2	2.09	0.53
1:A:348:ARG:O	1:A:352:MET:HB2	2.09	0.52
1:C:227:TRP:CZ3	1:C:251:VAL:HG11	2.44	0.52
1:D:433:GLU:HG2	4:D:2398:HOH:O	2.10	0.52
1:B:140:HIS:CG	1:B:368:GLN:HG3	2.45	0.52
1:C:279:ASP:HA	1:C:317:VAL:HG22	1.90	0.52
1:D:166:PHE:CE2	2:D:1446:CO8:H32	2.45	0.52
1:D:308:ASP:HA	1:D:327:ARG:HG2	1.92	0.51
1:B:433:GLU:HG2	1:B:440:ARG:HH22	1.75	0.51
1:B:287:ARG:HD2	4:B:2329:HOH:O	2.10	0.51
1:C:198:VAL:CG1	1:C:410:ALA:HB2	2.40	0.51
1:C:341:TYR:CD1	1:C:342:LEU:HD12	2.46	0.51
1:B:228:GLY:N	1:B:272[B]:ARG:HH22	1.93	0.51
1:C:69:VAL:HG13	1:C:117:CYS:HB2	1.93	0.51
1:A:227:TRP:CZ3	1:A:251:VAL:HG11	2.45	0.51
1:C:295:LEU:CD2	1:C:325:VAL:HG11	2.41	0.51
1:B:289:VAL:HA	1:B:324:ILE:HD13	1.93	0.50
1:B:95:GLN:HG2	1:B:98:ARG:NH1	2.27	0.50
1:C:271:ASN:O	1:C:274:GLU:HB2	2.11	0.50
1:C:69:VAL:HG11	1:C:172:GLY:O	2.11	0.50
1:A:351:TRP:O	1:D:361:HIS:HB2	2.11	0.50
1:C:271:ASN:O	1:C:274:GLU:CB	2.60	0.50
1:B:433:GLU:HG2	1:B:440:ARG:NH2	2.27	0.50
1:D:289:VAL:HA	1:D:324:ILE:HD13	1.92	0.50
1:D:66:LEU:HB3	1:D:123:ARG:HB2	1.94	0.50
1:C:146:GLU:HB3	1:D:146:GLU:HB3	1.92	0.50
1:A:93:LEU:HD11	1:A:111:HIS:CG	2.47	0.49
1:A:201:LEU:HD11	2:A:1446:CO8:H4'1	1.93	0.49
1:C:76:TYR:CE1	1:C:80:TRP:NE1	2.80	0.49
1:D:56:PRO:HD2	1:D:110:TYR:CZ	2.46	0.49
1:A:297:LYS:O	1:A:301:GLU:HG3	2.12	0.49
1:D:295:LEU:CG	1:D:325:VAL:HG11	2.42	0.49
1:B:180:ARG:HD3	4:B:2102:HOH:O	2.12	0.49
1:D:38:PHE:HB3	1:D:44:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:CB	1:C:107:ASP:HB2	2.42	0.49
1:D:426:ASP:HB2	4:D:2388:HOH:O	2.12	0.49
1:D:81:SER:HB2	1:D:89:THR:CG2	2.41	0.49
1:A:140:HIS:HB2	1:A:141:PRO:HD2	1.94	0.48
1:C:38:PHE:HB3	1:C:44:LYS:HG2	1.95	0.48
1:A:143:HIS:CG	1:A:168:THR:HG21	2.48	0.48
1:B:251:VAL:HG12	1:B:272[A]:ARG:HG3	1.94	0.48
1:A:146[A]:GLU:HB3	1:B:146:GLU:HG2	1.96	0.48
1:D:431:LEU:HD23	1:D:436:LEU:HD21	1.95	0.48
1:B:140:HIS:HB2	1:B:141:PRO:HD2	1.94	0.48
1:C:281:ILE:HG13	1:C:287:ARG:HG2	1.94	0.48
1:C:31:ARG:HG2	1:C:51:ARG:HD2	1.96	0.48
1:C:251:VAL:HG12	1:C:272:ARG:HG2	1.95	0.48
1:C:65:VAL:HG13	1:C:121:VAL:HG13	1.95	0.48
1:C:195:GLU:HB3	1:C:382:PRO:HG2	1.96	0.48
1:A:344:THR:HA	1:D:343:HIS:O	2.14	0.47
1:D:69:VAL:HG11	1:D:172:GLY:O	2.13	0.47
1:B:289:VAL:O	1:B:293[A]:ARG:HG3	2.13	0.47
1:A:69:VAL:HG13	1:A:117:CYS:HB2	1.96	0.47
1:C:287:ARG:HG3	4:C:2317:HOH:O	2.13	0.47
1:D:251:VAL:HG12	1:D:272:ARG:CG	2.44	0.47
1:D:143:HIS:CG	1:D:168:THR:HG21	2.49	0.47
1:A:33:GLU:HG2	4:A:2047:HOH:O	2.15	0.47
1:D:79:VAL:CG1	1:D:83:MET:HE1	2.45	0.47
1:A:74:ILE:HG21	1:A:397:CYS:HA	1.95	0.47
1:A:350:LEU:HD12	1:A:355:LYS:HB2	1.95	0.47
1:B:339:SER:HB3	3:B:1446:NAP:H2A	1.96	0.47
1:D:350:LEU:HD12	1:D:355:LYS:HB2	1.96	0.47
1:B:337:SER:HB3	1:B:341:TYR:HA	1.97	0.46
1:C:288:VAL:HG12	1:C:324:ILE:HD12	1.97	0.46
1:D:329:GLY:HA2	1:D:354:LEU:O	2.14	0.46
3:A:1447:NAP:H8A	3:A:1447:NAP:H3B	1.98	0.46
1:B:288:VAL:HG12	1:B:324:ILE:CD1	2.46	0.46
1:A:404:ARG:NH1	1:A:445:THR:HG21	2.30	0.46
1:B:69:VAL:HG11	1:B:172:GLY:O	2.15	0.46
1:C:198:VAL:HB	1:C:408:LYS:CB	2.46	0.46
1:A:94:LYS:HE2	4:A:2059:HOH:O	2.15	0.46
1:B:156:MET:HE2	1:B:361:HIS:O	2.15	0.46
1:C:321:LEU:O	1:C:325:VAL:HG13	2.16	0.46
1:A:75:ASN:OD1	1:A:201:LEU:HD22	2.15	0.46
1:B:8:LEU:HD22	1:B:416:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LYS:NZ	2:C:1446:CO8:H121	2.31	0.46
1:B:198:VAL:O	1:B:408:LYS:HE2	2.15	0.46
3:C:1445:NAP:H52A	3:C:1445:NAP:H52N	1.97	0.46
1:A:295:LEU:HG	1:A:325:VAL:HG21	1.97	0.45
1:A:288:VAL:HG12	1:A:324:ILE:HD12	1.97	0.45
1:B:285:PRO:CG	1:C:342:LEU:HD21	2.46	0.45
1:D:156:MET:HE2	1:D:361:HIS:O	2.16	0.45
1:C:30:LEU:HD21	1:C:82:ALA:HA	1.98	0.45
1:D:201:LEU:C	1:D:201:LEU:HD23	2.36	0.45
1:D:376:GLU:OE2	4:D:2207:HOH:O	2.21	0.45
1:B:295:LEU:HD23	1:B:325:VAL:CG1	2.39	0.45
1:D:140:HIS:HB2	1:D:141:PRO:HD2	1.98	0.45
1:A:26:LEU:HD11	1:A:52:LEU:HG	1.98	0.45
1:B:299:VAL:HG11	1:B:307:PRO:HD3	1.98	0.45
1:C:27:ALA:HB1	1:C:112:VAL:HG13	1.99	0.45
1:A:27:ALA:HB1	1:A:112:VAL:HG13	1.99	0.45
1:C:400:VAL:HA	1:C:405:GLN:OE1	2.17	0.45
1:D:353:LYS:HD2	4:D:2315:HOH:O	2.17	0.45
1:D:198:VAL:CG1	1:D:410:ALA:HB2	2.47	0.45
1:C:72:SER:HB3	1:C:173:LEU:HD23	1.99	0.45
1:B:343:HIS:O	1:C:344:THR:HA	2.17	0.45
1:D:79:VAL:O	1:D:83:MET:HG3	2.17	0.45
1:A:201:LEU:HD23	1:A:201:LEU:C	2.38	0.45
1:B:344:THR:HA	1:C:343:HIS:O	2.17	0.45
1:C:140:HIS:CG	1:C:368:GLN:HG3	2.52	0.45
2:A:1446:CO8:H2'1	3:A:1447:NAP:C7N	2.47	0.44
1:A:195:GLU:O	1:A:198:VAL:HG22	2.17	0.44
1:B:93:LEU:HD11	1:B:111:HIS:CG	2.52	0.44
1:C:273:ALA:O	1:C:274:GLU:C	2.55	0.44
1:D:257:LYS:HE3	1:D:444:ALA:HB1	1.97	0.44
1:C:361:HIS:CE1	2:C:1446:CO8:H5'1	2.53	0.44
1:B:326:ALA:HB3	1:B:355:LYS:HD3	1.98	0.44
1:B:47:ARG:HD2	4:B:2069:HOH:O	2.17	0.44
1:C:106:HIS:CE1	1:C:168:THR:HB	2.52	0.44
1:D:226:ILE:HA	1:D:311:PHE:HB3	1.98	0.44
1:A:146[A]:GLU:HG2	1:B:146:GLU:HB3	1.98	0.44
1:B:89:THR:HA	1:B:92:PHE:CD2	2.53	0.44
1:C:208:ARG:HG3	1:C:367:GLU:OE2	2.17	0.44
1:C:143:HIS:CG	1:C:168:THR:HG21	2.52	0.44
1:D:382:PRO:HB2	4:D:2354:HOH:O	2.18	0.44
1:D:198:VAL:HB	1:D:408:LYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LEU:HD11	1:C:111:HIS:CG	2.52	0.44
1:D:316:ARG:HB3	1:D:340:GLY:O	2.18	0.44
3:C:1445:NAP:C7N	2:C:1446:CO8:H2'1	2.48	0.43
1:A:153:GLY:HA3	1:B:366:GLU:OE1	2.17	0.43
1:A:126:ILE:HG13	1:B:62:PRO:HG3	1.99	0.43
1:D:146:GLU:H	1:D:146:GLU:CD	2.22	0.43
1:D:402:THR:OG1	1:D:404:ARG:HD2	2.17	0.43
1:B:195:GLU:HB3	1:B:382:PRO:HG2	2.00	0.43
1:B:257:LYS:HE3	1:B:444:ALA:HB1	1.99	0.43
1:C:201:LEU:HD23	1:C:201:LEU:C	2.39	0.43
1:C:351:TRP:CD1	1:C:351:TRP:C	2.91	0.43
1:C:67:VAL:O	1:C:176:TYR:HA	2.18	0.43
1:A:89:THR:HA	1:A:92:PHE:CD2	2.54	0.43
1:B:146:GLU:OE1	1:B:146:GLU:N	2.50	0.43
1:A:297:LYS:HG2	4:A:2381:HOH:O	2.17	0.43
1:B:361:HIS:CE1	2:B:1447:CO8:H5'1	2.54	0.43
1:B:44:LYS:HD2	1:B:85:GLU:OE2	2.19	0.43
1:C:116:ASP:O	1:C:117:CYS:HB3	2.18	0.43
1:C:335:CYS:HA	1:C:360:SER:O	2.18	0.43
1:D:287:ARG:HD2	4:D:2279:HOH:O	2.19	0.43
1:A:156:MET:HE2	1:A:361:HIS:O	2.19	0.43
1:B:198:VAL:HB	1:B:408:LYS:CB	2.49	0.43
1:B:356:LYS:HE2	4:B:2364:HOH:O	2.19	0.43
1:A:198:VAL:O	1:A:408:LYS:HE2	2.19	0.43
1:B:192:THR:HG21	1:B:419:GLY:HA2	2.00	0.43
3:C:1445:NAP:C4N	2:C:1446:CO8:H3'2	2.49	0.43
1:D:67:VAL:O	1:D:176:TYR:HA	2.19	0.43
1:A:69:VAL:HG11	1:A:172:GLY:O	2.19	0.43
1:C:70:MET:HG3	1:C:193:TRP:CE2	2.54	0.43
1:D:140:HIS:CG	1:D:368:GLN:HG3	2.54	0.43
1:A:237:ALA:O	1:A:241:VAL:HG23	2.19	0.42
1:C:257:LYS:HE3	1:C:444:ALA:HB1	2.01	0.42
1:C:269:VAL:O	1:C:302:LYS:HE3	2.18	0.42
1:D:242:LYS:HG2	1:D:248:PRO:HG3	2.00	0.42
1:A:281:ILE:HG13	1:A:287[A]:ARG:HG2	1.99	0.42
1:D:251:VAL:HG12	1:D:272:ARG:HG3	2.00	0.42
3:B:1446:NAP:C3B	3:B:1446:NAP:H8A	2.49	0.42
1:D:230:SER:HB2	1:D:406:VAL:HG22	2.00	0.42
1:B:350:LEU:HD21	1:C:357:ILE:HG22	2.02	0.42
1:D:288:VAL:HG12	1:D:324:ILE:HD12	2.02	0.42
1:B:285:PRO:HG3	1:C:342:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:HB	1:C:408:LYS:HB3	2.01	0.42
1:B:226:ILE:HA	1:B:311:PHE:HB3	2.02	0.42
1:D:69:VAL:HG13	1:D:117:CYS:HB2	2.01	0.42
1:C:126:ILE:HG13	1:D:62:PRO:HG3	2.02	0.42
1:A:318:THR:HA	1:A:321:LEU:HD12	2.02	0.41
3:B:1446:NAP:H52N	3:B:1446:NAP:H52A	2.01	0.41
1:B:337:SER:CB	1:B:341:TYR:HA	2.50	0.41
1:B:351:TRP:CD1	1:B:351:TRP:C	2.94	0.41
1:A:353:LYS:NZ	2:D:1446:CO8:H121	2.35	0.41
1:C:381:VAL:HG11	1:C:435:ARG:HD3	2.01	0.41
1:A:430:ARG:NH1	4:A:2504:HOH:O	2.53	0.41
1:C:139:VAL:HG21	1:C:179:VAL:HG11	2.02	0.41
1:C:286:ARG:NE	4:C:2313:HOH:O	2.54	0.41
1:C:180:ARG:HD3	4:C:2120:HOH:O	2.20	0.41
1:C:349:TYR:O	1:C:355:LYS:HE3	2.21	0.41
3:D:1445:NAP:C7N	2:D:1446:CO8:H2'1	2.50	0.41
1:D:297:LYS:HA	1:D:297:LYS:HD3	1.53	0.41
1:A:257:LYS:NZ	3:A:1447:NAP:O3X	2.41	0.41
1:A:257:LYS:HE3	1:A:444:ALA:HB1	2.02	0.41
1:C:237:ALA:O	1:C:241:VAL:HG23	2.20	0.41
1:C:326:ALA:HB3	1:C:355:LYS:HD3	2.03	0.41
1:D:216:ALA:HB1	1:D:309:ILE:HG12	2.01	0.41
1:C:30:LEU:O	1:C:110:TYR:HA	2.21	0.41
1:C:7:VAL:CG1	1:C:70:MET:HE3	2.51	0.41
1:D:131:TRP:CZ3	1:D:137:VAL:HG12	2.56	0.41
1:D:252:VAL:HA	3:D:1445:NAP:O1X	2.20	0.41
1:A:351:TRP:CD1	1:A:351:TRP:C	2.94	0.41
1:B:361:HIS:HB2	1:C:351:TRP:O	2.21	0.41
1:A:58:PRO:HG2	1:A:178:VAL:HG21	2.02	0.41
1:D:295:LEU:HD23	1:D:325:VAL:HG11	2.03	0.41
1:D:93:LEU:HD11	1:D:111:HIS:CG	2.55	0.41
1:A:366:GLU:OE1	1:B:153:GLY:HA3	2.21	0.41
1:B:143:HIS:CG	1:B:168:THR:HG21	2.56	0.41
1:D:251:VAL:CG1	1:D:272:ARG:HG2	2.51	0.41
1:D:291:THR:HA	1:D:294:LYS:HE3	2.03	0.41
1:B:352:MET:HG3	2:C:1446:CO8:CEP	2.51	0.40
1:A:26:LEU:HB3	1:A:175:GLU:HG3	2.02	0.40
1:C:381:VAL:HG11	1:C:435:ARG:CD	2.51	0.40
1:C:89:THR:HA	1:C:92:PHE:CD2	2.56	0.40
1:A:226:ILE:HA	1:A:311:PHE:HB3	2.03	0.40
1:A:361:HIS:HB2	1:D:351:TRP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:CYS:HA	1:D:360:SER:O	2.22	0.40
1:A:116:ASP:O	1:A:117:CYS:HB3	2.21	0.40
1:B:233:LEU:HD12	3:B:1446:NAP:H51N	2.03	0.40
1:C:251:VAL:HG12	1:C:272:ARG:CG	2.52	0.40
1:C:251:VAL:CG1	1:C:272:ARG:HG2	2.52	0.40
1:D:138:ILE:HG23	1:D:187:LYS:HA	2.03	0.40
1:A:339:SER:HB3	3:A:1447:NAP:H2A	2.03	0.40
1:C:270:ILE:HG23	1:C:298:LEU:HD23	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	446/447 (100%)	433 (97%)	12 (3%)	1 (0%)	51	41
1	B	445/447 (100%)	433 (97%)	11 (2%)	1 (0%)	51	41
1	C	444/447 (99%)	429 (97%)	14 (3%)	1 (0%)	51	41
1	D	442/447 (99%)	427 (97%)	13 (3%)	2 (0%)	32	20
All	All	1777/1788 (99%)	1722 (97%)	50 (3%)	5 (0%)	44	34

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%)	71	69
1	B	350/350 (100%)	344 (98%)	6 (2%)	66	62
1	C	349/350 (100%)	344 (99%)	5 (1%)	71	69
1	D	347/350 (99%)	340 (98%)	7 (2%)	60	55
All	All	1397/1400 (100%)	1374 (98%)	23 (2%)	66	65

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
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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
1	B	217	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	-	52,59,59	2.16	10 (19%)	59,85,85	2.01	10 (16%)
3	NAP	A	1447	-	44,52,52	1.58	4 (9%)	51,80,80	2.04	11 (21%)
3	NAP	B	1446	-	44,52,52	1.46	6 (13%)	51,80,80	1.75	5 (9%)
2	CO8	B	1447	-	52,59,59	1.92	7 (13%)	59,85,85	1.72	5 (8%)
3	NAP	C	1445	-	44,52,52	1.55	7 (15%)	51,80,80	2.57	9 (17%)
2	CO8	C	1446	-	52,59,59	2.03	10 (19%)	59,85,85	1.77	7 (11%)
3	NAP	D	1445	-	44,52,52	1.69	7 (15%)	51,80,80	2.84	17 (33%)
2	CO8	D	1446	-	52,59,59	1.93	6 (11%)	59,85,85	1.86	8 (13%)

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	-	-	0/54/74/74	0/3/3/3
3	NAP	A	1447	-	-	0/27/67/67	0/5/5/5
3	NAP	B	1446	-	-	0/27/67/67	0/5/5/5
2	CO8	B	1447	-	-	0/54/74/74	0/3/3/3
3	NAP	C	1445	-	-	0/27/67/67	0/5/5/5
2	CO8	C	1446	-	-	0/54/74/74	0/3/3/3
3	NAP	D	1445	-	-	0/27/67/67	0/5/5/5
2	CO8	D	1446	-	-	2/54/74/74	0/3/3/3

All (57) 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
2	A	1446	CO8	C3'-C2'	-3.80	1.38	1.52
2	B	1447	CO8	C3'-C2'	-3.70	1.38	1.52
2	C	1446	CO8	C3'-C2'	-3.43	1.39	1.52
2	D	1446	CO8	C3'-C2'	-3.39	1.39	1.52
3	C	1445	NAP	C2D-C1D	-2.43	1.49	1.53
2	C	1446	CO8	C4'-C3'	-2.16	1.39	1.51
2	A	1446	CO8	C6P-C5P	2.00	1.55	1.51
3	B	1446	NAP	PA-O1A	2.03	1.58	1.50
2	B	1447	CO8	OAP-CAP	2.03	1.46	1.42
3	C	1445	NAP	PN-O1N	2.05	1.58	1.50
2	C	1446	CO8	C6P-C5P	2.06	1.55	1.51
2	B	1447	CO8	O1'-C1'	2.12	1.24	1.21
2	C	1446	CO8	O1'-C1'	2.14	1.24	1.21
2	C	1446	CO8	P3B-O3B	2.16	1.63	1.59
3	C	1445	NAP	O4B-C1B	2.32	1.44	1.41
2	A	1446	CO8	OAP-CAP	2.33	1.46	1.42
3	C	1445	NAP	C6N-N1N	2.36	1.41	1.35
3	D	1445	NAP	O4D-C1D	2.36	1.44	1.41
2	A	1446	CO8	P2A-O4A	2.46	1.60	1.50
2	B	1447	CO8	P3B-O9A	2.49	1.65	1.54
3	B	1446	NAP	O4D-C4D	2.50	1.50	1.45
2	A	1446	CO8	P3B-O8A	2.50	1.65	1.54
3	D	1445	NAP	C6N-N1N	2.52	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1446	CO8	O1'-C1'	2.55	1.24	1.21
3	B	1446	NAP	P2B-O1X	2.63	1.59	1.50
2	D	1446	CO8	P2A-O4A	2.82	1.61	1.50
3	B	1446	NAP	C6N-N1N	2.83	1.42	1.35
3	A	1447	NAP	C6N-N1N	2.97	1.43	1.35
2	C	1446	CO8	P1A-O1A	3.04	1.62	1.50
3	D	1445	NAP	PN-O1N	3.06	1.62	1.50
2	C	1446	CO8	P2A-O4A	3.18	1.62	1.50
3	C	1445	NAP	P2B-O2X	3.22	1.68	1.54
3	D	1445	NAP	P2B-O2X	3.24	1.68	1.54
2	B	1447	CO8	P2A-O4A	3.36	1.63	1.50
3	B	1446	NAP	P2B-O2B	3.36	1.65	1.59
2	D	1446	CO8	P1A-O1A	3.37	1.63	1.50
3	A	1447	NAP	O4D-C1D	3.48	1.46	1.41
2	D	1446	CO8	P3B-O7A	3.51	1.62	1.50
2	C	1446	CO8	P3B-O7A	3.53	1.62	1.50
2	A	1446	CO8	P3B-O7A	3.71	1.63	1.50
3	A	1447	NAP	P2B-O1X	3.71	1.63	1.50
2	A	1446	CO8	O4B-C1B	4.00	1.46	1.41
2	A	1446	CO8	P1A-O1A	4.08	1.66	1.50
3	D	1445	NAP	O4B-C1B	4.35	1.47	1.41
2	D	1446	CO8	O4B-C1B	4.35	1.47	1.41
2	B	1447	CO8	O4B-C1B	4.53	1.47	1.41
3	C	1445	NAP	P2B-O1X	4.54	1.66	1.50
3	B	1446	NAP	O4B-C1B	5.02	1.48	1.41
3	D	1445	NAP	P2B-O1X	5.11	1.68	1.50
2	C	1446	CO8	O4B-C1B	5.25	1.48	1.41
3	D	1445	NAP	P2B-O2B	5.33	1.68	1.59
3	C	1445	NAP	P2B-O2B	5.90	1.69	1.59
3	A	1447	NAP	O4B-C1B	6.51	1.50	1.41

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1445	NAP	N3A-C2A-N1A	-10.97	119.31	128.86
3	C	1445	NAP	O3X-P2B-O1X	-9.63	72.81	110.50
3	B	1446	NAP	N3A-C2A-N1A	-9.51	120.57	128.86
3	D	1445	NAP	O3X-P2B-O2X	-9.13	70.78	107.61
3	C	1445	NAP	N3A-C2A-N1A	-8.97	121.04	128.86
2	A	1446	CO8	N3A-C2A-N1A	-8.76	121.22	128.86
2	C	1446	CO8	N3A-C2A-N1A	-8.62	121.35	128.86
2	B	1447	CO8	N3A-C2A-N1A	-8.61	121.36	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1446	CO8	N3A-C2A-N1A	-8.41	121.53	128.86
3	A	1447	NAP	N3A-C2A-N1A	-7.66	122.19	128.86
3	C	1445	NAP	O3X-P2B-O2X	-6.84	80.03	107.61
3	D	1445	NAP	O3X-P2B-O1X	-6.21	86.19	110.50
2	A	1446	CO8	C2P-C3P-N4P	-5.13	101.17	112.49
3	D	1445	NAP	O3X-P2B-O2B	-4.99	83.31	106.00
3	A	1447	NAP	C3N-C7N-N7N	-4.64	112.48	117.77
3	D	1445	NAP	C3N-C7N-N7N	-4.60	112.52	117.77
3	A	1447	NAP	C3N-C2N-N1N	-4.50	115.90	120.43
3	A	1447	NAP	C4D-O4D-C1D	-4.46	105.02	109.77
3	C	1445	NAP	O3X-P2B-O2B	-4.45	85.75	106.00
3	C	1445	NAP	C3N-C7N-N7N	-4.21	112.97	117.77
2	D	1446	CO8	O1'-C1'-S1P	-3.66	119.00	122.84
3	A	1447	NAP	O2B-P2B-O1X	-3.36	96.11	109.26
2	C	1446	CO8	O1'-C1'-S1P	-3.31	119.38	122.84
3	D	1445	NAP	C5B-C4B-C3B	-3.06	103.64	115.29
3	A	1447	NAP	O3D-C3D-C4D	-2.72	103.14	111.09
3	D	1445	NAP	O4B-C4B-C5B	-2.66	100.43	109.40
3	D	1445	NAP	C4D-O4D-C1D	-2.64	106.96	109.77
3	B	1446	NAP	C4D-O4D-C1D	-2.59	107.01	109.77
3	D	1445	NAP	C3N-C2N-N1N	-2.44	117.97	120.43
3	B	1446	NAP	C3N-C7N-N7N	-2.41	115.02	117.77
2	B	1447	CO8	C6'-C5'-C4'	-2.35	102.36	114.45
2	D	1446	CO8	C7P-C6P-C5P	-2.26	108.59	112.22
2	A	1446	CO8	O8A-P3B-O7A	-2.19	101.94	110.50
2	A	1446	CO8	C7P-C6P-C5P	-2.18	108.72	112.22
2	A	1446	CO8	O5P-C5P-N4P	-2.15	118.86	122.97
3	C	1445	NAP	C1B-N9A-C4A	-2.15	122.92	126.64
2	D	1446	CO8	C2P-S1P-C1'	-2.14	94.81	101.90
2	C	1446	CO8	O1'-C1'-C2'	-2.13	122.08	123.95
3	D	1445	NAP	C1B-N9A-C4A	-2.12	122.97	126.64
2	A	1446	CO8	C1B-N9A-C4A	-2.10	123.00	126.64
2	D	1446	CO8	C2P-C3P-N4P	-2.09	107.88	112.49
3	A	1447	NAP	C1B-N9A-C4A	-2.04	123.11	126.64
3	A	1447	NAP	O7N-C7N-C3N	2.01	121.97	119.62
3	D	1445	NAP	O2N-PN-O1N	2.05	122.89	112.28
3	A	1447	NAP	O7N-C7N-N7N	2.06	125.51	122.58
2	C	1446	CO8	O6A-CCP-CBP	2.06	113.86	110.55
2	A	1446	CO8	CDP-CBP-CAP	2.08	112.43	108.82
3	D	1445	NAP	O5D-PN-O1N	2.12	117.81	109.25
2	B	1447	CO8	C4'-C3'-C2'	2.21	121.33	113.24
3	D	1445	NAP	C2A-N1A-C6A	2.38	122.94	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1445	NAP	O2N-PN-O5D	2.39	119.44	108.14
3	C	1445	NAP	O7N-C7N-C3N	2.42	122.46	119.62
3	B	1446	NAP	C2A-N1A-C6A	2.45	123.05	118.77
3	A	1447	NAP	O3X-P2B-O2X	2.49	117.67	107.61
3	D	1445	NAP	O7N-C7N-N7N	2.53	126.18	122.58
2	A	1446	CO8	C6P-C5P-N4P	2.54	120.88	116.49
2	B	1447	CO8	CEP-CBP-CAP	2.62	113.36	108.82
2	D	1446	CO8	C4'-C3'-C2'	2.66	122.98	113.24
3	B	1446	NAP	N6A-C6A-N1A	2.73	124.17	118.77
3	D	1445	NAP	O2X-P2B-O1X	3.00	122.23	110.50
2	C	1446	CO8	C4'-C3'-C2'	3.04	124.40	113.24
3	C	1445	NAP	O2B-P2B-O1X	3.05	121.23	109.26
3	D	1445	NAP	O2X-P2B-O2B	3.67	122.69	106.00
3	D	1445	NAP	C2N-C3N-C4N	3.69	122.48	118.26
2	C	1446	CO8	C3'-C2'-C1'	3.72	118.61	113.12
3	A	1447	NAP	C2N-C3N-C4N	3.90	122.71	118.26
2	A	1446	CO8	C3P-N4P-C5P	3.97	130.47	122.84
2	D	1446	CO8	C2'-C1'-S1P	4.30	117.61	113.28
2	C	1446	CO8	C2'-C1'-S1P	5.22	118.54	113.28
2	D	1446	CO8	C3'-C2'-C1'	5.96	121.92	113.12
2	B	1447	CO8	C3'-C2'-C1'	6.03	122.02	113.12
2	A	1446	CO8	C3'-C2'-C1'	6.82	123.20	113.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1446	CO8	O1'-C1'-S1P-C2P
2	D	1446	CO8	C2'-C1'-S1P-C2P

There are no ring outliers.

8 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1446	CO8	2	0
3	A	1447	NAP	7	0
3	B	1446	NAP	9	0
2	B	1447	CO8	4	0
3	C	1445	NAP	6	0
2	C	1446	CO8	5	0
3	D	1445	NAP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1446	CO8	5	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	445/447 (99%)	0.63	15 (3%) 46 49	14, 20, 36, 46	1 (0%)
1	B	445/447 (99%)	0.61	19 (4%) 36 39	13, 20, 37, 47	1 (0%)
1	C	444/447 (99%)	0.44	17 (3%) 41 45	13, 21, 38, 58	3 (0%)
1	D	444/447 (99%)	0.73	33 (7%) 15 17	15, 23, 41, 58	0
All	All	1778/1788 (99%)	0.60	84 (4%) 32 36	13, 21, 39, 58	5 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	282	ALA	5.2
1	C	276	GLY	5.2
1	D	53	GLY	4.8
1	B	275	LEU	4.7
1	D	275	LEU	4.1
1	C	273	ALA	4.1
1	C	80	TRP	4.0
1	D	76	TYR	3.7
1	A	274	GLU	3.4
1	C	87	ILE	3.3
1	A	275	LEU	3.3
1	C	274	GLU	3.2
1	B	210	LEU	3.1
1	B	286	ARG	3.1
1	B	290	GLU	3.1
1	B	211	VAL	3.1
1	D	87	ILE	3.0
1	C	281	ILE	3.0
1	A	13	ALA	3.0
1	C	278	THR	2.9
1	C	76	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	273	ALA	2.8
1	A	354	LEU	2.7
1	C	435	ARG	2.7
1	A	211	VAL	2.7
1	B	274	GLU	2.7
1	D	157	LEU	2.6
1	A	286	ARG	2.6
1	D	144	VAL	2.6
1	D	1	SER	2.6
1	D	309	ILE	2.6
1	A	41	VAL	2.6
1	D	153	GLY	2.6
1	C	150	ALA	2.6
1	A	207	TYR	2.5
1	A	273	ALA	2.5
1	A	363	ALA	2.5
1	B	363	ALA	2.5
1	B	207	TYR	2.5
1	D	276	GLY	2.5
1	B	209	MET	2.5
1	C	36	ASP	2.4
1	A	157	LEU	2.4
1	D	435	ARG	2.4
1	D	332	VAL	2.4
1	D	279	ASP	2.4
1	B	157	LEU	2.4
1	D	363	ALA	2.4
1	B	142	ALA	2.4
1	D	9	ASP	2.4
1	B	203	ALA	2.3
1	D	156	MET	2.3
1	D	151	THR	2.3
1	D	233	LEU	2.3
1	D	80	TRP	2.3
1	D	211	VAL	2.3
1	C	286	ARG	2.3
1	D	142	ALA	2.3
1	D	150	ALA	2.3
1	C	279	ASP	2.3
1	D	40	GLY	2.2
1	B	273	ALA	2.2
1	D	216	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	430	ARG	2.2
1	B	139	VAL	2.2
1	D	274	GLU	2.2
1	B	185	LEU	2.2
1	D	152	HIS	2.2
1	B	216	ALA	2.2
1	C	153	GLY	2.2
1	C	283	ASP	2.1
1	D	205	THR	2.1
1	A	357	ILE	2.1
1	C	151	THR	2.1
1	D	36	ASP	2.1
1	B	215	GLY	2.1
1	A	309	ILE	2.1
1	B	205	THR	2.0
1	D	207	TYR	2.0
1	B	241	VAL	2.0
1	A	210	LEU	2.0
1	C	434	ASP	2.0
1	A	331	THR	2.0
1	D	212	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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
2	CO8	C	1446	57/57	0.59	0.37	4.52	11,78,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO8	D	1446	57/57	0.69	0.30	2.96	7,50,68,68	0
2	CO8	B	1447	57/57	0.82	0.24	2.33	6,31,46,46	0
2	CO8	A	1446	57/57	0.88	0.22	2.30	2,27,40,41	0
3	NAP	C	1445	48/48	0.92	0.17	1.58	10,18,25,27	0
3	NAP	D	1445	48/48	0.93	0.14	-0.37	10,15,23,23	0
3	NAP	B	1446	48/48	0.96	0.10	-1.53	2,9,16,17	0
3	NAP	A	1447	48/48	0.95	0.10	-1.93	2,8,14,16	0

## 6.5 Other polymers

There are no such residues in this entry.