Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:55 PM GMT

PDB ID	:	4DPL
Title	:	Structure of malonyl-coenzyme A reductase from crenarchaeota in complex with NadP
Authors	:	Demmer, U.; Warkentin, E; Srivastava, A.; Kockelkorn, D.; Fuchs, G.; Ermler, U.
Deposited on	:	2012-02-13
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

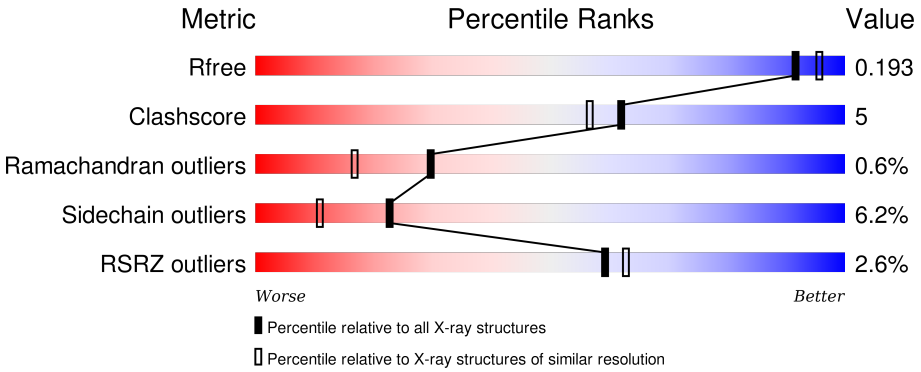
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	2% 84% 13%
1	B	359	2% 86% 10%
1	C	359	3% 85% 12%
1	D	359	4% 84% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	B	401	-	-	-	X
3	UNL	A	402	-	-	-	X
3	UNL	B	402	-	-	X	X
3	UNL	C	402	-	-	X	X
3	UNL	D	402	-	-	-	X

2 Entry composition

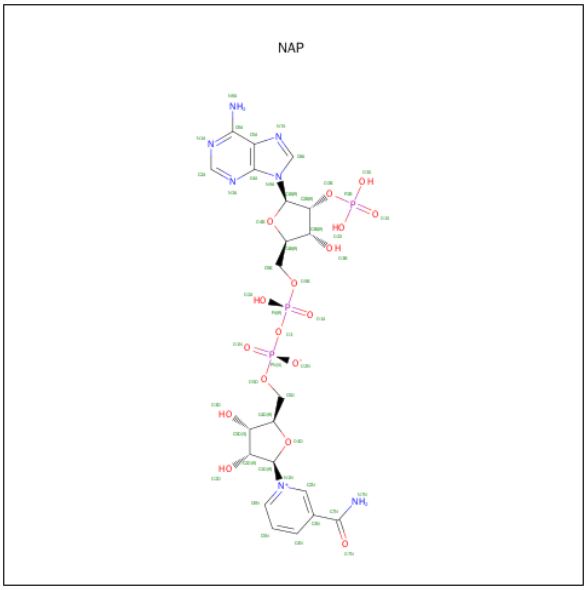
There are 4 unique types of molecules in this entry. The entry contains 12082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Malonyl-CoA/succinyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	1	0
			2746	1761	466	510	9			
1	B	354	Total	C	N	O	S	0	2	0
			2749	1763	466	511	9			
1	C	353	Total	C	N	O	S	0	1	0
			2738	1757	463	510	8			
1	D	354	Total	C	N	O	S	0	1	0
			2746	1761	466	510	9			

- 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 UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

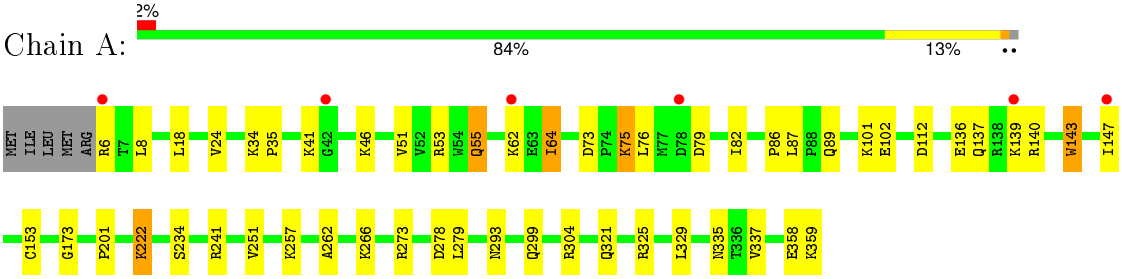
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total	O	0	0
			233	233		
4	B	225	Total	O	0	0
			225	225		
4	C	245	Total	O	0	0
			245	245		
4	D	184	Total	O	0	0
			184	184		

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 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.

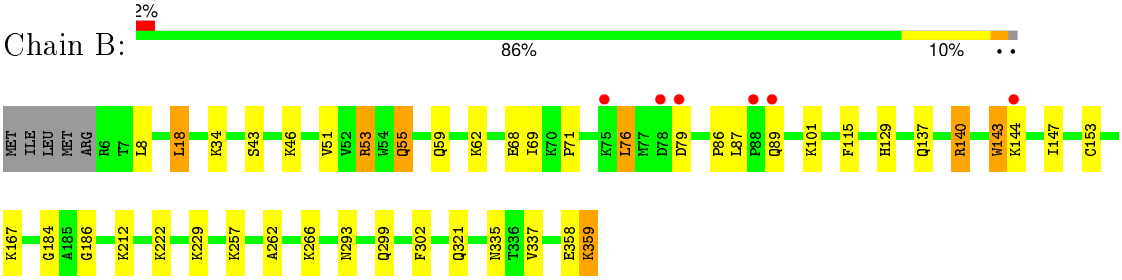
- Molecule 1: Malonyl-CoA/succinyl-CoA reductase

Chain A:



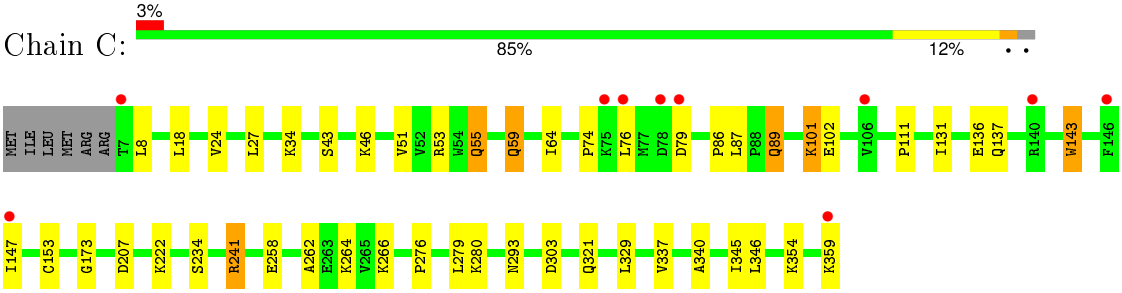
- Molecule 1: Malonyl-CoA/succinyl-CoA reductase

Chain B:



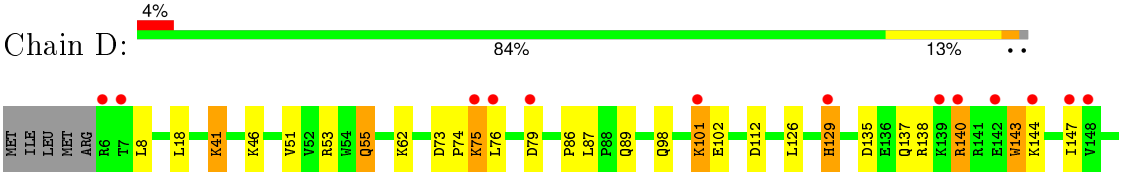
- Molecule 1: Malonyl-CoA/succinyl-CoA reductase

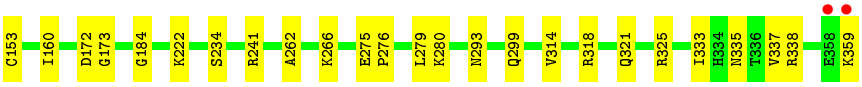
Chain C:



- Molecule 1: Malonyl-CoA/succinyl-CoA reductase

Chain D:




C153
I160
D172
G173
G184
K222
S234
R241
A262
K266
E275
P276
L279
K280
N293
Q299
V314
R318
Q321
R325
I333
H334
N335
T336
V337
R338
E358
K359

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.58Å 128.80Å 140.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.90) 99.5 (19.95-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.163 , 0.194 0.162 , 0.193	Depositor DCC
R_{free} test set	6787 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 134386 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, UNL

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	1.01	1/2810 (0.0%)	0.90	5/3816 (0.1%)
1	B	0.99	1/2816 (0.0%)	0.86	2/3824 (0.1%)
1	C	0.98	0/2802	0.89	5/3806 (0.1%)
1	D	0.93	3/2810 (0.1%)	0.85	5/3816 (0.1%)
All	All	0.98	5/11238 (0.0%)	0.87	17/15262 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	ARG	CZ-NH1	8.54	1.44	1.33
1	D	135	ASP	C-O	7.65	1.37	1.23
1	A	251	VAL	CB-CG2	5.78	1.65	1.52
1	D	314	VAL	CB-CG1	5.69	1.64	1.52
1	B	302	PHE	CE1-CZ	5.20	1.47	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	241	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	C	241	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	241	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	241	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	D	318	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	B	53	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	325	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	D	138	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	C	18	LEU	CA-CB-CG	-6.38	100.62	115.30
1	B	18	LEU	CA-CB-CG	-6.29	100.83	115.30
1	A	18	LEU	CA-CB-CG	-5.77	102.03	115.30
1	C	207	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	18	LEU	CA-CB-CG	-5.39	102.90	115.30
1	C	303	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	172	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	304	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	241	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	2746	0	2803	29	0
1	B	2749	0	2808	29	0
1	C	2738	0	2793	33	0
1	D	2746	0	2803	29	0
2	A	48	0	25	0	0
2	B	48	0	25	3	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
3	A	6	0	0	1	0
3	B	6	0	0	2	0
3	C	6	0	0	3	0
3	D	6	0	0	1	0
4	A	233	0	0	2	0
4	B	225	0	0	1	0
4	C	245	0	0	5	0
4	D	184	0	0	3	0
All	All	12082	0	11307	120	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 5.

All (120) 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:A:8:LEU:HD13	1:A:82:ILE:HD11	1.39	1.03
1:D:137:GLN:HE22	1:D:147:ILE:H	1.20	0.89
1:A:262:ALA:H	1:A:321:GLN:HE22	1.19	0.89
1:A:137:GLN:HE22	1:A:147:ILE:H	1.22	0.87
1:B:262:ALA:H	1:B:321:GLN:HE22	1.25	0.84
1:B:137:GLN:HE22	1:B:147:ILE:H	1.27	0.83
1:C:262:ALA:H	1:C:321:GLN:HE22	1.29	0.79
1:A:262:ALA:H	1:A:321:GLN:NE2	1.78	0.79
1:B:266:LYS:NZ	1:B:293:ASN:ND2	2.31	0.78
1:D:262:ALA:H	1:D:321:GLN:HE22	1.30	0.78
1:C:137:GLN:HE21	1:C:143:TRP:HE1	1.34	0.75
1:C:59[A]:GLN:HG3	4:C:521:HOH:O	1.87	0.74
1:C:137:GLN:HE22	1:C:147:ILE:H	1.34	0.72
1:A:53:ARG:HH12	1:A:55:GLN:HE21	1.38	0.71
1:D:137:GLN:HE21	1:D:143:TRP:HE1	1.37	0.70
1:B:262:ALA:H	1:B:321:GLN:NE2	1.88	0.70
1:C:258:GLU:OE1	4:C:610:HOH:O	2.10	0.69
1:D:262:ALA:H	1:D:321:GLN:NE2	1.92	0.68
1:D:53:ARG:HH12	1:D:55:GLN:HE21	1.41	0.67
1:C:34:LYS:NZ	4:C:532:HOH:O	2.28	0.67
1:A:46:LYS:HD3	1:A:51:VAL:HG11	1.77	0.65
1:A:137:GLN:HE21	1:A:143:TRP:HE1	1.41	0.65
1:C:46:LYS:HD3	1:C:51:VAL:HG11	1.75	0.65
1:A:8:LEU:HD13	1:A:82:ILE:CD1	2.23	0.65
1:B:212:LYS:NZ	4:B:723:HOH:O	2.26	0.65
1:A:8:LEU:HD21	1:A:358:GLU:O	1.97	0.65
1:B:266:LYS:HZ1	1:B:293:ASN:ND2	1.93	0.64
1:A:266:LYS:NZ	1:A:293:ASN:ND2	2.47	0.63
1:C:101:LYS:HE2	1:C:143:TRP:HE3	1.64	0.62
1:C:8:LEU:HD21	1:C:359:LYS:HA	1.80	0.62
1:B:8:LEU:HD21	1:B:359:LYS:HA	1.79	0.62
1:B:51:VAL:HG21	1:B:69:ILE:CD1	2.30	0.62
1:A:53:ARG:HH12	1:A:55:GLN:NE2	1.98	0.61
1:A:73:ASP:OD1	1:A:75:LYS:HG2	2.01	0.60
1:C:266:LYS:NZ	1:C:293:ASN:ND2	2.50	0.60
1:C:53:ARG:HH12	1:C:55:GLN:HE21	1.49	0.59
1:D:53:ARG:HH12	1:D:55:GLN:NE2	1.99	0.59
1:D:153[B]:CYS:HB3	3:D:402:UNL:C1	2.32	0.59
1:C:262:ALA:H	1:C:321:GLN:NE2	1.99	0.58
1:B:71:PRO:HG2	1:B:76:LEU:HD23	1.85	0.58
1:D:75:LYS:N	1:D:75:LYS:HD2	2.20	0.57
1:B:153[B]:CYS:HB3	3:B:402:UNL:C1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:HH22	1:A:55:GLN:HE22	1.53	0.57
1:B:266:LYS:HZ2	1:B:293:ASN:ND2	2.03	0.56
1:C:153:CYS:SG	3:C:402:UNL:C1	2.91	0.56
1:A:262:ALA:N	1:A:321:GLN:HE22	1.98	0.55
1:A:153[B]:CYS:HB3	3:A:402:UNL:C1	2.36	0.55
1:D:41:LYS:HB3	2:D:401:NAP:O2X	2.07	0.54
1:A:153[B]:CYS:SG	1:A:335:ASN:HA	2.48	0.54
1:C:53:ARG:HH12	1:C:55:GLN:NE2	2.06	0.54
1:B:53:ARG:HH12	1:B:55:GLN:HE21	1.56	0.53
1:B:266:LYS:HZ2	1:B:293:ASN:HD22	1.55	0.53
1:A:139:LYS:HE2	4:A:717:HOH:O	2.08	0.52
1:D:73:ASP:OD1	1:D:75:LYS:HG2	2.10	0.52
1:A:75:LYS:HE3	1:A:102:GLU:OE1	2.10	0.52
1:C:266:LYS:HZ3	1:C:293:ASN:HD21	1.57	0.52
1:B:71:PRO:HG2	1:B:76:LEU:CD2	2.40	0.52
1:B:137:GLN:HE21	1:B:143:TRP:HE1	1.57	0.51
1:C:89:GLN:HB2	1:C:111:PRO:HG2	1.91	0.51
1:D:266:LYS:NZ	1:D:293:ASN:ND2	2.58	0.51
1:A:266:LYS:HZ2	1:A:293:ASN:ND2	2.08	0.51
1:C:24:VAL:HG13	1:C:64:ILE:HD13	1.92	0.51
1:D:153[B]:CYS:SG	1:D:335:ASN:HA	2.51	0.50
1:A:299:GLN:HA	4:A:660:HOH:O	2.10	0.50
1:C:266:LYS:HZ1	1:C:293:ASN:ND2	2.08	0.50
1:B:266:LYS:NZ	1:B:293:ASN:HD21	2.09	0.50
1:D:275:GLU:N	1:D:276:PRO:CD	2.75	0.50
1:D:137:GLN:HE22	1:D:147:ILE:N	1.99	0.49
1:C:153:CYS:SG	3:C:402:UNL:O	2.71	0.49
1:C:53:ARG:HH22	1:C:55:GLN:HE22	1.60	0.49
2:B:401:NAP:C5N	3:B:402:UNL:O	2.60	0.49
1:D:325:ARG:HG3	1:D:325:ARG:HH11	1.78	0.49
1:C:241:ARG:NH1	3:C:402:UNL:O41	2.30	0.49
1:C:24:VAL:HG13	1:C:64:ILE:HG21	1.96	0.48
1:C:101:LYS:HE3	1:C:101:LYS:HB2	1.51	0.47
1:D:173:GLY:HA2	1:D:234:SER:O	2.15	0.47
1:B:53:ARG:HH12	1:B:55:GLN:NE2	2.13	0.47
1:C:266:LYS:NZ	1:C:293:ASN:HD21	2.12	0.47
1:C:173:GLY:HA2	1:C:234:SER:O	2.15	0.46
1:D:75:LYS:HE3	1:D:102:GLU:OE1	2.16	0.46
1:C:74:PRO:HB2	1:C:102:GLU:HG3	1.97	0.46
1:A:222:LYS:HB2	1:A:222:LYS:HE3	1.52	0.46
1:A:266:LYS:HZ1	1:A:293:ASN:ND2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ARG:HH22	1:D:55:GLN:HE22	1.64	0.46
1:B:262:ALA:N	1:B:321:GLN:HE22	2.05	0.45
1:C:137:GLN:HE22	1:C:147:ILE:N	2.09	0.45
1:D:89:GLN:NE2	4:D:643:HOH:O	2.49	0.45
1:B:51:VAL:HG21	1:B:69:ILE:HD12	1.98	0.45
1:A:273:ARG:NH2	1:A:278:ASP:OD1	2.43	0.45
1:D:140:ARG:HB2	1:D:140:ARG:HH11	1.82	0.45
1:D:126:LEU:HD11	1:D:160:ILE:HA	2.00	0.44
1:A:24:VAL:HG13	1:A:64:ILE:HD12	1.99	0.44
1:D:129:HIS:HB2	4:D:588:HOH:O	2.17	0.44
1:B:153[B]:CYS:SG	1:B:335:ASN:HA	2.58	0.44
1:A:35:PRO:HG2	1:A:64:ILE:HD11	1.99	0.44
1:A:173:GLY:HA2	1:A:234:SER:O	2.18	0.44
1:C:89:GLN:NE2	4:C:615:HOH:O	2.50	0.43
1:B:18:LEU:HD12	1:B:186:GLY:HA2	2.00	0.43
1:A:266:LYS:HZ2	1:A:293:ASN:HD22	1.64	0.43
4:C:680:HOH:O	1:D:299:GLN:HA	2.19	0.43
1:C:74:PRO:CB	1:C:102:GLU:HG3	2.49	0.43
1:B:184:GLY:HA2	2:B:401:NAP:C7N	2.48	0.43
1:A:137:GLN:HE22	1:A:147:ILE:N	2.03	0.42
1:D:184:GLY:HA2	2:D:401:NAP:O7N	2.19	0.42
1:A:201:PRO:HD3	1:B:299:GLN:HG2	2.01	0.42
1:B:115:PHE:CZ	1:B:212:LYS:HG2	2.55	0.42
1:B:140:ARG:HB3	1:B:140:ARG:NH1	2.34	0.42
1:C:276:PRO:HB3	1:C:346:LEU:HD11	2.02	0.42
1:D:46:LYS:HD3	1:D:51:VAL:HG11	2.02	0.42
1:C:27:LEU:HD21	1:C:345:ILE:HG12	2.03	0.41
1:D:8:LEU:HD21	1:D:359:LYS:HA	2.03	0.41
1:B:137:GLN:NE2	1:B:147:ILE:H	2.07	0.41
1:C:131:ILE:HD11	1:C:354:LYS:HG3	2.03	0.41
1:B:184:GLY:HA2	2:B:401:NAP:O7N	2.20	0.41
1:D:333:ILE:HD11	1:D:338:ARG:HG3	2.02	0.41
1:D:101:LYS:NZ	1:D:101:LYS:HB2	2.36	0.41
1:B:59:GLN:HG3	4:D:612:HOH:O	2.21	0.40
1:C:43:SER:OG	2:C:401:NAP:O1X	2.28	0.40
1:D:262:ALA:N	1:D:321:GLN:HE22	2.07	0.40
1:B:140:ARG:CB	1:B:140:ARG:HH11	2.34	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	353/359 (98%)	344 (98%)	7 (2%)	2 (1%)	30 17
1	B	354/359 (99%)	343 (97%)	9 (2%)	2 (1%)	30 17
1	C	352/359 (98%)	341 (97%)	8 (2%)	3 (1%)	21 9
1	D	353/359 (98%)	340 (96%)	11 (3%)	2 (1%)	30 17
All	All	1412/1436 (98%)	1368 (97%)	35 (2%)	9 (1%)	30 17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	B	86	PRO
1	C	86	PRO
1	D	86	PRO
1	C	340	ALA
1	D	337	VAL
1	B	337	VAL
1	A	337	VAL
1	C	337	VAL

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	298/302 (99%)	277 (93%)	21 (7%)	19 8
1	B	299/302 (99%)	278 (93%)	21 (7%)	19 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	297/302 (98%)	282 (95%)	15 (5%)	29 17
1	D	298/302 (99%)	280 (94%)	18 (6%)	24 12
All	All	1192/1208 (99%)	1117 (94%)	75 (6%)	23 10

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	34	LYS
1	A	41	LYS
1	A	55	GLN
1	A	62	LYS
1	A	64	ILE
1	A	75	LYS
1	A	76	LEU
1	A	79	ASP
1	A	87	LEU
1	A	89	GLN
1	A	101	LYS
1	A	112	ASP
1	A	136	GLU
1	A	140	ARG
1	A	143	TRP
1	A	222	LYS
1	A	257	LYS
1	A	279	LEU
1	A	329	LEU
1	A	359	LYS
1	B	34	LYS
1	B	43	SER
1	B	46	LYS
1	B	55	GLN
1	B	62	LYS
1	B	68	GLU
1	B	76	LEU
1	B	79	ASP
1	B	87	LEU
1	B	89	GLN
1	B	101	LYS
1	B	129	HIS
1	B	140	ARG

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Mol	Chain	Res	Type
1	B	143	TRP
1	B	144	LYS
1	B	167	LYS
1	B	222	LYS
1	B	229	LYS
1	B	257	LYS
1	B	358	GLU
1	B	359	LYS
1	C	55	GLN
1	C	59[A]	GLN
1	C	59[B]	GLN
1	C	76	LEU
1	C	79	ASP
1	C	87	LEU
1	C	89	GLN
1	C	101	LYS
1	C	136	GLU
1	C	143	TRP
1	C	222	LYS
1	C	264	LYS
1	C	279	LEU
1	C	280	LYS
1	C	329	LEU
1	D	41	LYS
1	D	55	GLN
1	D	62	LYS
1	D	74	PRO
1	D	75	LYS
1	D	76	LEU
1	D	79	ASP
1	D	87	LEU
1	D	98	GLN
1	D	101	LYS
1	D	112	ASP
1	D	129	HIS
1	D	140	ARG
1	D	143	TRP
1	D	144	LYS
1	D	222	LYS
1	D	279	LEU
1	D	280	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	129	HIS
1	A	137	GLN
1	A	180	GLN
1	A	293	ASN
1	A	321	GLN
1	B	55	GLN
1	B	137	GLN
1	B	180	GLN
1	B	293	ASN
1	B	321	GLN
1	C	55	GLN
1	C	129	HIS
1	C	137	GLN
1	C	180	GLN
1	C	293	ASN
1	C	321	GLN
1	D	55	GLN
1	D	137	GLN
1	D	180	GLN
1	D	293	ASN
1	D	321	GLN

5.3.3 RNA

There are no RNA molecules 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

Of 8 ligands modelled in this entry, 4 are unknown - leaving 4 for Mogul analysis.

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	-	42,52,52	1.55	4 (9%)	54,80,80	2.10	10 (18%)
2	NAP	B	401	-	42,52,52	1.48	3 (7%)	54,80,80	1.87	8 (14%)
2	NAP	C	401	-	42,52,52	1.47	3 (7%)	54,80,80	2.02	9 (16%)
2	NAP	D	401	-	42,52,52	1.26	3 (7%)	54,80,80	1.81	5 (9%)

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
2	NAP	B	401	-	-	0/27/67/67	0/5/5/5
2	NAP	C	401	-	-	0/27/67/67	0/5/5/5
2	NAP	D	401	-	-	0/27/67/67	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	C3N-C7N	-6.72	1.39	1.50
2	C	401	NAP	C3N-C7N	-6.19	1.40	1.50
2	B	401	NAP	C3N-C7N	-5.88	1.41	1.50
2	D	401	NAP	C3N-C7N	-5.30	1.42	1.50
2	A	401	NAP	C2A-N3A	2.03	1.35	1.32
2	D	401	NAP	O4D-C1D	2.09	1.43	1.41
2	D	401	NAP	O4B-C1B	2.67	1.44	1.41
2	B	401	NAP	O4D-C1D	3.09	1.45	1.41
2	B	401	NAP	O4B-C1B	3.22	1.45	1.41
2	C	401	NAP	O4D-C1D	3.50	1.45	1.41
2	C	401	NAP	O4B-C1B	3.54	1.45	1.41
2	A	401	NAP	O4D-C1D	3.75	1.45	1.41
2	A	401	NAP	O4B-C1B	3.82	1.46	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	NAP	N3A-C2A-N1A	-11.72	119.92	128.89
2	A	401	NAP	N3A-C2A-N1A	-10.64	120.75	128.89
2	D	401	NAP	N3A-C2A-N1A	-10.27	121.03	128.89
2	B	401	NAP	N3A-C2A-N1A	-9.42	121.68	128.89
2	A	401	NAP	C3N-C7N-N7N	-2.76	114.79	117.82
2	B	401	NAP	O3-PN-O5D	-2.70	95.77	102.94
2	B	401	NAP	C3N-C7N-N7N	-2.70	114.86	117.82
2	D	401	NAP	C4A-C5A-N7A	-2.62	107.07	109.48
2	C	401	NAP	C1B-N9A-C4A	-2.36	123.38	126.94
2	C	401	NAP	C3N-C7N-N7N	-2.34	115.25	117.82
2	A	401	NAP	PN-O3-PA	-2.18	126.59	132.73
2	B	401	NAP	C4A-C5A-N7A	-2.15	107.50	109.48
2	C	401	NAP	O5D-PN-O1N	-2.10	101.45	109.62
2	A	401	NAP	O3-PN-O5D	-2.07	97.44	102.94
2	A	401	NAP	O2N-PN-O3	2.00	114.18	105.09
2	D	401	NAP	O2N-PN-O3	2.07	114.46	105.09
2	C	401	NAP	O2N-PN-O1N	2.07	123.72	112.53
2	C	401	NAP	O2N-PN-O3	2.07	114.48	105.09
2	C	401	NAP	C2A-N1A-C6A	2.10	122.52	118.77
2	A	401	NAP	C2B-C3B-C4B	2.11	106.85	101.85
2	B	401	NAP	O2N-PN-O3	2.26	115.34	105.09
2	D	401	NAP	O3X-P2B-O1X	2.28	117.92	110.58
2	A	401	NAP	O7N-C7N-N7N	2.30	125.83	122.59
2	B	401	NAP	C2B-C3B-C4B	2.58	107.96	101.85
2	C	401	NAP	O3X-P2B-O1X	2.60	118.94	110.58
2	A	401	NAP	O3X-P2B-O2X	2.82	118.12	107.38
2	A	401	NAP	O2X-P2B-O1X	2.96	120.10	110.58
2	D	401	NAP	O4D-C1D-N1N	3.07	111.50	108.13
2	C	401	NAP	O4D-C1D-N1N	3.10	111.53	108.13
2	B	401	NAP	O7N-C7N-N7N	3.15	127.02	122.59
2	B	401	NAP	O4D-C1D-N1N	3.80	112.31	108.13
2	A	401	NAP	O4D-C1D-N1N	6.48	115.25	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAP	3	0
2	C	401	NAP	1	0
2	D	401	NAP	2	0

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	354/359 (98%)	-0.34	6 (1%)	73	76	16, 28, 59, 84	0
1	B	354/359 (98%)	-0.28	6 (1%)	73	76	15, 30, 58, 83	0
1	C	353/359 (98%)	-0.23	10 (2%)	56	60	16, 29, 58, 98	0
1	D	354/359 (98%)	-0.10	15 (4%)	40	44	17, 35, 67, 89	0
All	All	1415/1436 (98%)	-0.24	37 (2%)	59	63	15, 30, 62, 98	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	78	ASP	6.6
1	A	6	ARG	5.5
1	D	6	ARG	5.4
1	C	76	LEU	5.2
1	C	75	LYS	4.4
1	C	79	ASP	4.2
1	C	359	LYS	4.0
1	D	358	GLU	3.9
1	D	139	LYS	3.5
1	B	144	LYS	3.4
1	C	106	VAL	3.3
1	D	140	ARG	3.2
1	D	147	ILE	3.1
1	D	359	LYS	3.0
1	B	78	ASP	3.0
1	D	75	LYS	3.0
1	C	147	ILE	2.9
1	D	142	GLU	2.7
1	D	148	VAL	2.6
1	B	79	ASP	2.5
1	C	146	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	7	THR	2.5
1	B	75	LYS	2.5
1	D	7	THR	2.4
1	D	76	LEU	2.4
1	D	144	LYS	2.4
1	A	42	GLY	2.3
1	A	139	LYS	2.3
1	B	89	GLN	2.3
1	D	129	HIS	2.3
1	A	147	ILE	2.3
1	D	79	ASP	2.2
1	C	140	ARG	2.2
1	A	78	ASP	2.1
1	B	88	PRO	2.1
1	A	62	LYS	2.0
1	D	101	LYS	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^{th} 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^2)	Q<0.9
3	UNL	D	402	6/-	0.89	0.15	7.31	33,40,48,50	0
3	UNL	C	402	6/-	0.90	0.14	4.69	33,37,43,59	0
3	UNL	A	402	6/-	0.91	0.11	3.20	31,35,41,44	0
3	UNL	B	402	6/-	0.87	0.14	3.20	36,40,41,43	0
2	NAP	B	401	48/48	0.84	0.25	2.90	30,62,84,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAP	A	401	48/48	0.91	0.17	1.81	31,52,63,69	0
2	NAP	D	401	48/48	0.92	0.18	1.77	35,59,73,90	0
2	NAP	C	401	48/48	0.93	0.14	0.98	29,45,56,67	0

6.5 Other polymers (i)

There are no such residues in this entry.