W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 11:01 PM GMT

PDB ID	:	1W6U
Title	:	STRUCTURE OF HUMAN DECR TERNARY COMPLEX
Authors	:	Alphey, M.S.; Byres, E.; Li, D.; Hunter, W.N.
Deposited on	:	2004-08-24
Resolution	:	1.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 (i)) were used in the production of this report:

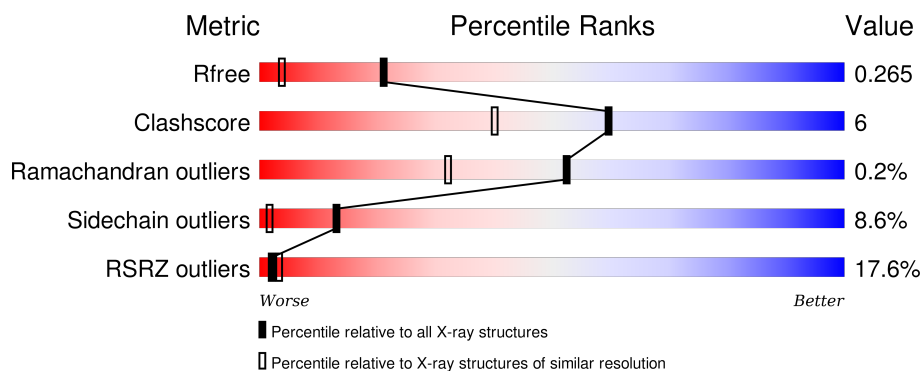|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.75 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		8.6%
RSRZ outliers		17.6%

Worse　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	302	15% / 80% 14% • 5%
1	B	302	14% / 82% 11% • 5%
1	C	302	19% / 77% 16% • 5%
1	D	302	18% / 78% 14% • 7%

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	HXC	A	1330	-	-	-	X
3	HXC	B	1331	-	-	-	X
3	HXC	C	1330	-	-	-	X
3	HXC	D	1329	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9640 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 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	6	0
			2171	1375	370	415	11			
1	B	286	Total	C	N	O	S	0	6	0
			2162	1368	368	414	12			
1	C	286	Total	C	N	O	S	0	6	0
			2158	1367	365	415	11			
1	D	282	Total	C	N	O	S	0	2	0
			2125	1348	359	406	12			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
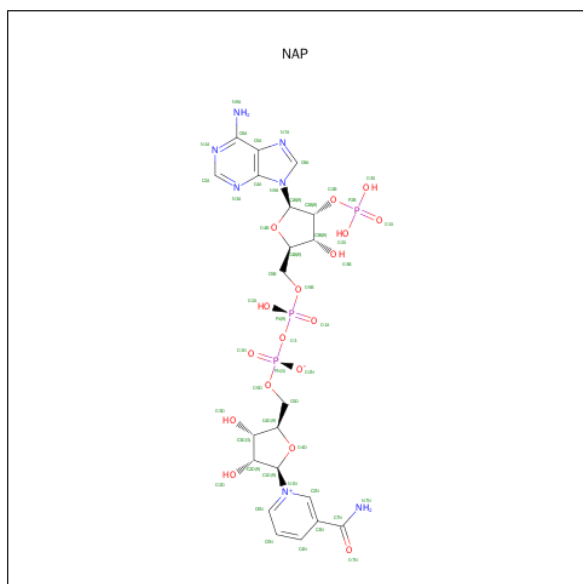
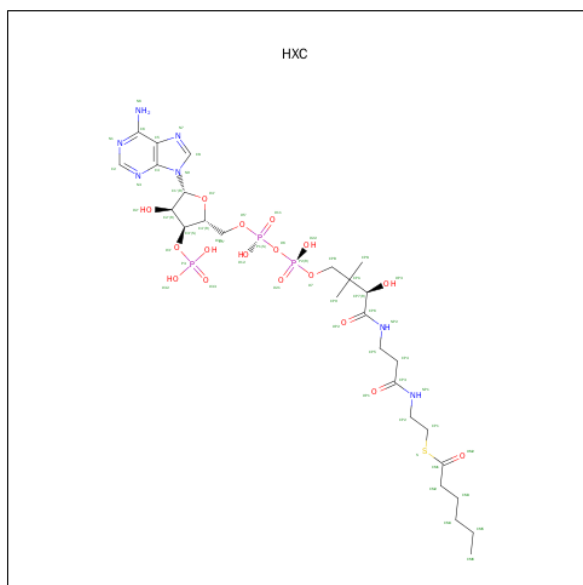| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			56	23	7	21	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	1
			56	23	7	21	5		
2	C	1	Total	C	N	O	P	0	1
			56	23	7	21	5		
2	D	1	Total	C	N	O	P	0	1
			56	23	7	21	5		

- Molecule 3 is HEXANOYL-COENZYME A (three-letter code: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total	O	0	0
			138	138		
4	B	149	Total	O	0	0
			149	149		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	131	Total 131	O 131	0	0
4	D	162	Total 162	O 162	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
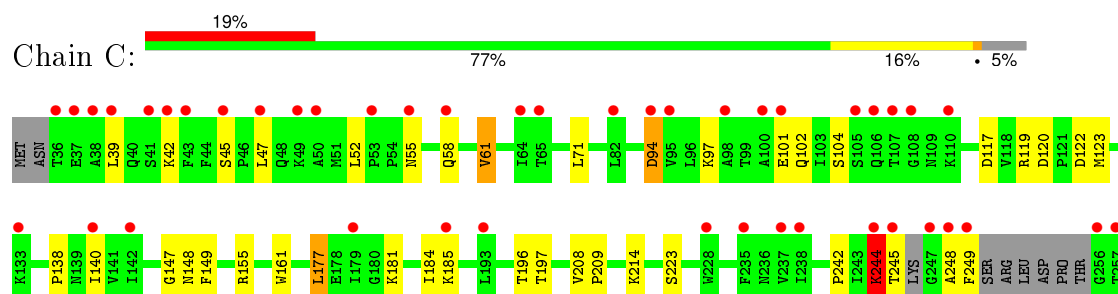
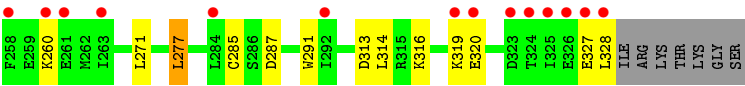- Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR
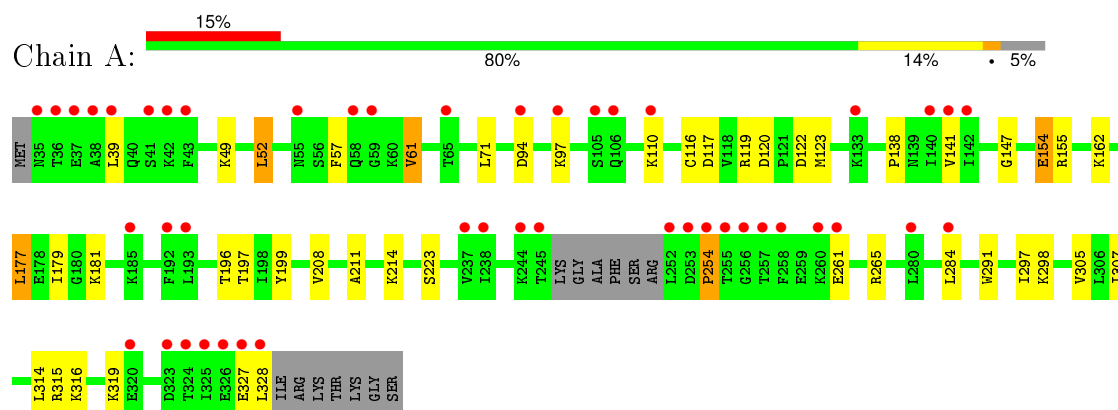
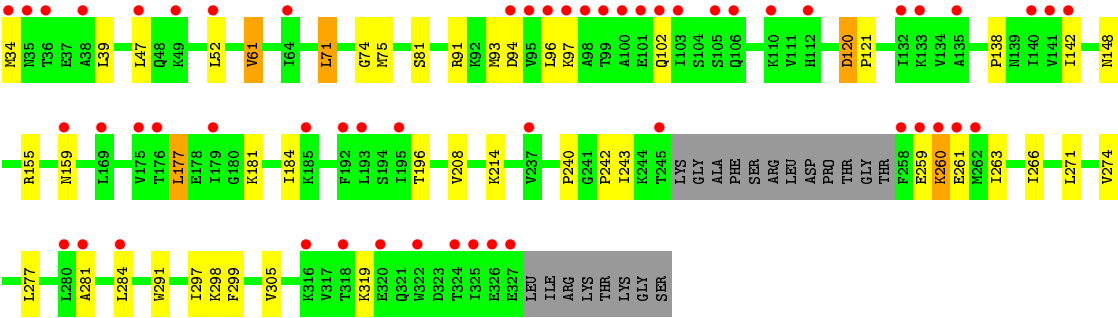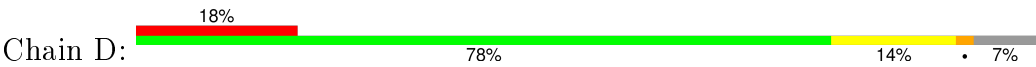- Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR
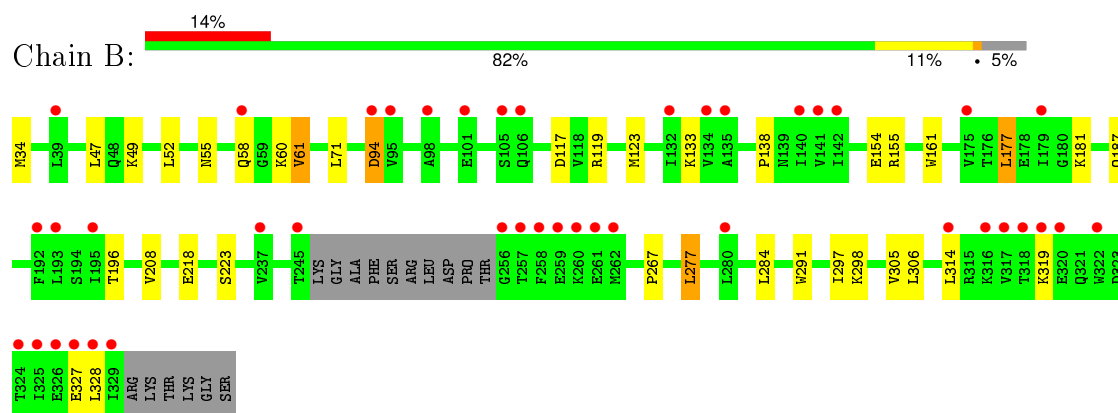
- Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR

● Molecule 1: 2,4-DIENOYL-COA REDUCTASE, MITOCHONDRIAL PRECURSOR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.28Å 131.66Å 70.85Å 90.00° 92.64° 90.00°	Depositor
Resolution (Å)	70.71 – 1.75 29.52 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.3 (70.71-1.75) 95.3 (29.52-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.227 , 0.268 0.225 , 0.265	Depositor DCC
R_{free} test set	5590 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.877	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.6	EDS
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 110710 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9640	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HXC, 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	0.38	0/2232	0.66	5/3019 (0.2%)
1	B	0.37	0/2224	0.64	3/3006 (0.1%)
1	C	0.35	0/2218	0.64	6/2998 (0.2%)
1	D	0.35	0/2169	0.63	2/2932 (0.1%)
All	All	0.37	0/8843	0.64	16/11955 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	94	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	254	PRO	N-CA-CB	5.84	110.31	103.30
1	C	120	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	122	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	287	ASP	CB-CG-OD2	5.43	123.19	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2171	0	2181	22	0
1	B	2162	0	2184	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2158	0	2174	28	0
1	D	2125	0	2151	26	0
2	A	56	0	10	0	0
2	B	56	0	10	1	0
2	C	56	0	10	2	0
2	D	56	0	10	0	0
3	A	55	0	42	3	0
3	B	55	0	42	5	0
3	C	55	0	42	20	0
3	D	55	0	42	8	0
4	A	138	0	0	1	0
4	B	149	0	0	1	0
4	C	131	0	0	3	0
4	D	162	0	0	7	0
All	All	9640	0	8898	103	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 6.

The worst 5 of 103 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)
3:D:1329:HXC:HP11	3:D:1329:HXC:HM32	1.12	1.07
3:C:1330:HXC:HP81	3:C:1330:HXC:HP2	1.21	1.05
1:C:148:ASN:H	3:C:1330:HXC:HP52	1.27	0.99
3:D:1329:HXC:HP11	3:D:1329:HXC:CM3	1.96	0.92
1:A:154:GLU:HG2	1:C:184:ILE:HD13	1.50	0.91

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	290/302 (96%)	281 (97%)	8 (3%)	1 (0%)	46	25
1	B	288/302 (95%)	281 (98%)	7 (2%)	0	100	100
1	C	286/302 (95%)	279 (98%)	6 (2%)	1 (0%)	46	25
1	D	280/302 (93%)	272 (97%)	8 (3%)	0	100	100
All	All	1144/1208 (95%)	1113 (97%)	29 (2%)	2 (0%)	52	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	PRO
1	C	244	LYS

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	233/243 (96%)	216 (93%)	17 (7%)	17	3
1	B	234/243 (96%)	214 (92%)	20 (8%)	13	2
1	C	233/243 (96%)	205 (88%)	28 (12%)	6	0
1	D	229/243 (94%)	214 (93%)	15 (7%)	21	4
All	All	929/972 (96%)	849 (91%)	80 (9%)	13	2

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	328	LEU
1	C	94[B]	ASP
1	D	155	ARG
1	C	39	LEU
1	C	47	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	126	ASN
1	B	182	GLN
1	C	321	GLN
1	B	55	ASN
1	C	126	ASN

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 ⓘ

12 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	1329[A]	-	42,52,52	1.54	3 (7%)	54,80,80	1.95	4 (7%)
2	NAP	A	1329[B]	-	42,52,52	1.54	3 (7%)	54,80,80	1.87	3 (5%)
3	HXC	A	1330	-	47,57,57	2.37	10 (21%)	59,83,83	2.65	13 (22%)
2	NAP	B	1330[A]	-	42,52,52	1.55	3 (7%)	54,80,80	1.93	5 (9%)
2	NAP	B	1330[B]	-	42,52,52	1.54	3 (7%)	54,80,80	1.83	3 (5%)
3	HXC	B	1331	-	47,57,57	2.39	9 (19%)	59,83,83	2.88	17 (28%)
2	NAP	C	1329[A]	-	42,52,52	1.52	3 (7%)	54,80,80	1.93	3 (5%)
2	NAP	C	1329[B]	-	42,52,52	1.52	3 (7%)	54,80,80	1.88	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	HXC	C	1330	-	47,57,57	2.36	10 (21%)	59,83,83	2.79	12 (20%)
2	NAP	D	1328[A]	-	42,52,52	1.55	3 (7%)	54,80,80	1.93	4 (7%)
2	NAP	D	1328[B]	-	42,52,52	1.55	3 (7%)	54,80,80	1.85	4 (7%)
3	HXC	D	1329	-	47,57,57	2.33	9 (19%)	59,83,83	3.32	14 (23%)

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	1329[A]	-	-	0/27/67/67	0/5/5/5
2	NAP	A	1329[B]	-	-	0/27/67/67	0/5/5/5
3	HXC	A	1330	-	-	2/52/72/72	0/3/3/3
2	NAP	B	1330[A]	-	-	0/27/67/67	0/5/5/5
2	NAP	B	1330[B]	-	-	0/27/67/67	0/5/5/5
3	HXC	B	1331	-	-	3/52/72/72	0/3/3/3
2	NAP	C	1329[A]	-	-	0/27/67/67	0/5/5/5
2	NAP	C	1329[B]	-	-	0/27/67/67	0/5/5/5
3	HXC	C	1330	-	-	2/52/72/72	0/3/3/3
2	NAP	D	1328[A]	-	-	0/27/67/67	0/5/5/5
2	NAP	D	1328[B]	-	-	0/27/67/67	0/5/5/5
3	HXC	D	1329	-	-	3/52/72/72	0/3/3/3

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1330	HXC	CM2-CM1	-9.76	1.39	1.50
3	B	1331	HXC	CM2-CM1	-9.53	1.40	1.50
3	D	1329	HXC	CM2-CM1	-9.22	1.40	1.50
3	C	1330	HXC	CM2-CM1	-8.97	1.40	1.50
3	C	1330	HXC	CP4-CP3	-5.92	1.39	1.51

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1329[B]	NAP	N3A-C2A-N1A	-11.98	119.72	128.89
2	A	1329[A]	NAP	N3A-C2A-N1A	-11.98	119.72	128.89
2	C	1329[A]	NAP	N3A-C2A-N1A	-11.93	119.76	128.89
2	C	1329[B]	NAP	N3A-C2A-N1A	-11.93	119.76	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1330[B]	NAP	N3A-C2A-N1A	-11.75	119.89	128.89

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1331	HXC	CP1-CP2-NP1-CP3
3	D	1329	HXC	CM2-CM1-S-CP1
3	D	1329	HXC	OM2-CM1-S-CP1
3	C	1330	HXC	CM2-CM1-S-CP1
3	C	1330	HXC	OM2-CM1-S-CP1

There are no ring outliers.

6 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1330	HXC	3	0
2	B	1330[B]	NAP	1	0
3	B	1331	HXC	5	0
2	C	1329[B]	NAP	2	0
3	C	1330	HXC	20	0
3	D	1329	HXC	8	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	288/302 (95%)	0.83	46 (15%)	3	4	17, 26, 59, 77	0
1	B	286/302 (94%)	0.91	42 (14%)	3	5	17, 27, 56, 74	0
1	C	286/302 (94%)	1.11	58 (20%)	1	2	19, 33, 63, 82	0
1	D	282/302 (93%)	1.08	55 (19%)	1	2	21, 33, 56, 75	0
All	All	1142/1208 (94%)	0.98	201 (17%)	2	3	17, 30, 59, 82	0

The worst 5 of 201 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ILE	13.4
1	B	258	PHE	13.1
1	D	258	PHE	9.3
1	B	257	THR	8.7
1	C	328	LEU	8.1

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, 95th 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	HXC	D	1329	55/55	0.62	0.36	4.03	75,77,79,79	45
3	HXC	C	1330	55/55	0.44	0.45	3.10	78,84,86,86	45
3	HXC	B	1331	55/55	0.57	0.34	2.90	77,79,82,82	45
3	HXC	A	1330	55/55	0.60	0.33	2.82	81,83,84,84	45
2	NAP	C	1329[B]	48/48	0.93	0.12	0.28	37,39,41,42	8
2	NAP	A	1329[A]	48/48	0.94	0.13	0.28	27,30,34,36	8
2	NAP	A	1329[B]	48/48	0.94	0.13	0.28	27,30,32,34	8
2	NAP	B	1330[B]	48/48	0.93	0.11	-0.01	29,33,36,37	8
2	NAP	B	1330[A]	48/48	0.93	0.11	-0.01	29,33,36,37	8
2	NAP	D	1328[B]	48/48	0.90	0.12	-0.13	34,37,41,42	8
2	NAP	D	1328[A]	48/48	0.90	0.12	-0.13	34,37,41,42	8
2	NAP	C	1329[A]	48/48	0.93	0.12	-0.20	37,39,43,43	8

6.5 Other polymers (i)

There are no such residues in this entry.