



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:02 PM GMT

PDB ID : 1DQA
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH HMG, COA, AND NADP+
Authors : Istvan, E.S.; Palnitkar, M.; Buchanan, S.K.; Deisenhofer, J.
Deposited on : 1999-12-30
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

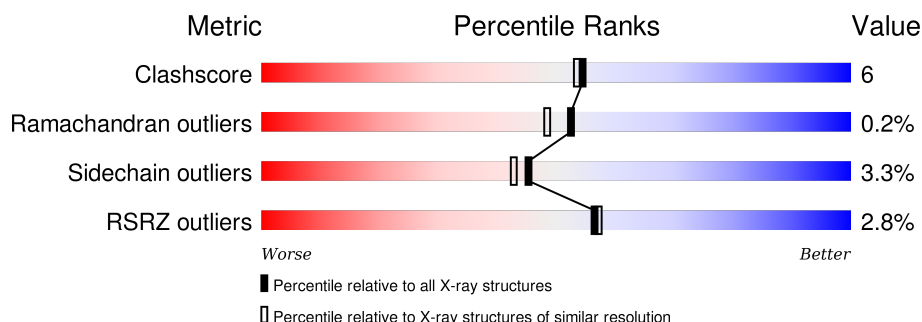
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	467	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>12%</div> </div> </div>
1	B	467	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>13%</div> </div> </div>
1	C	467	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>13%</div> </div> </div>
1	D	467	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>15%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	A	101	X	-	-	-
2	COA	B	102	X	-	-	-
2	COA	C	103	X	-	-	-
2	COA	D	104	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12909 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.

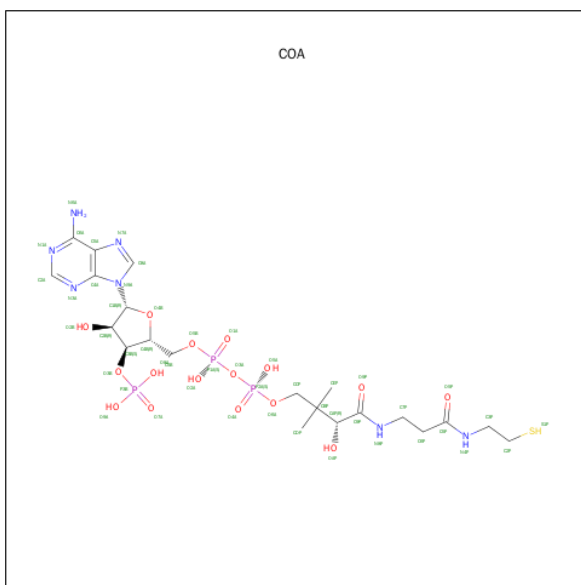
- Molecule 1 is a protein called PROTEIN (HMG-COA REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3044	1897	537	580	30			
1	B	405	Total	C	N	O	S	0	0	0
			3010	1876	530	575	29			
1	C	404	Total	C	N	O	S	0	0	0
			3011	1876	535	570	30			
1	D	396	Total	C	N	O	S	0	0	0
			2945	1832	522	561	30			

There are 4 discrepancies between the modelled and reference sequences:

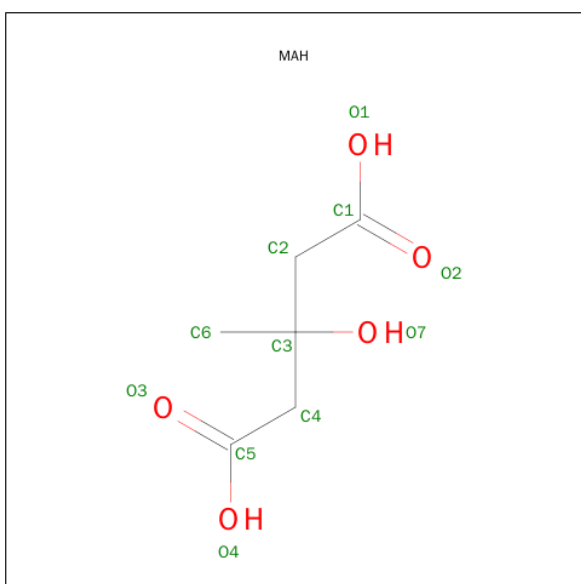
Chain	Residue	Modelled	Actual	Comment	Reference
A	485	ILE	MET	MUTATION	UNP P04035
B	485	ILE	MET	MUTATION	UNP P04035
C	485	ILE	MET	MUTATION	UNP P04035
D	485	ILE	MET	MUTATION	UNP P04035

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



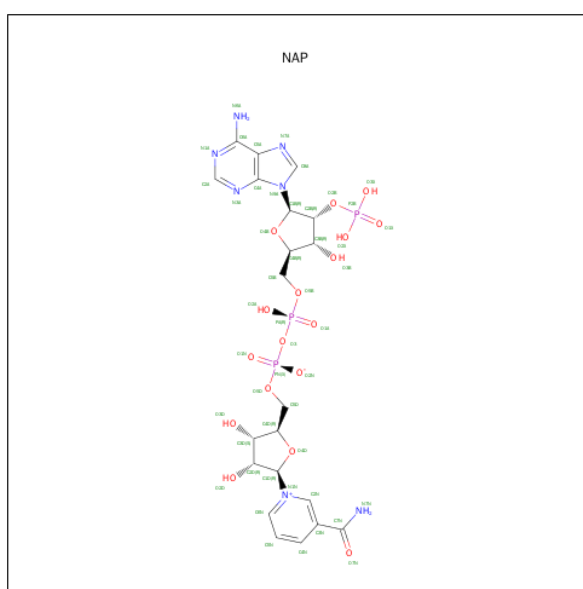
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 3 is 3-HYDROXY-3-METHYL-GLUTARIC ACID (three-letter code: MAH) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		

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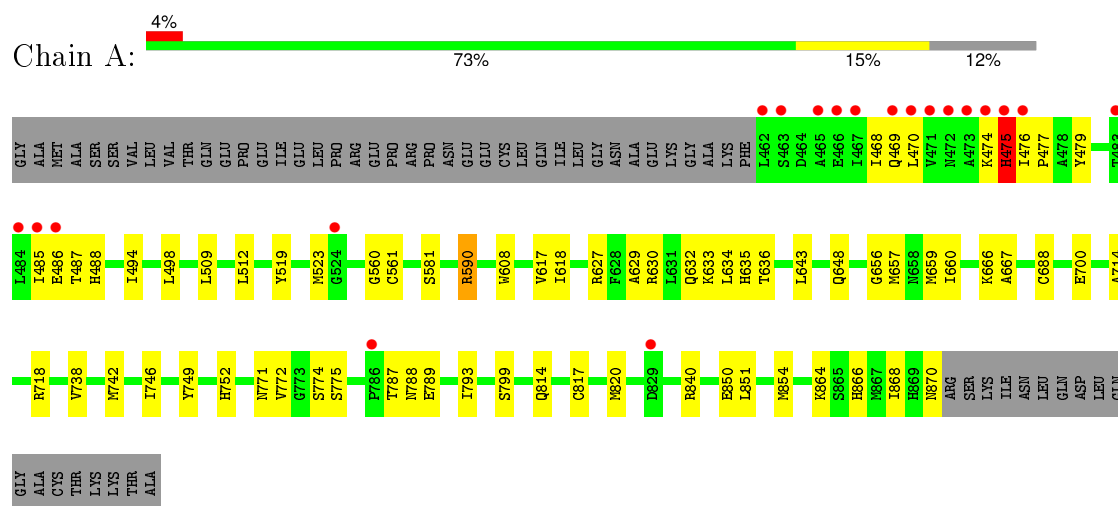
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	119	Total 119	O 119	0	0
5	C	106	Total 106	O 106	0	0
5	D	125	Total 125	O 125	0	0

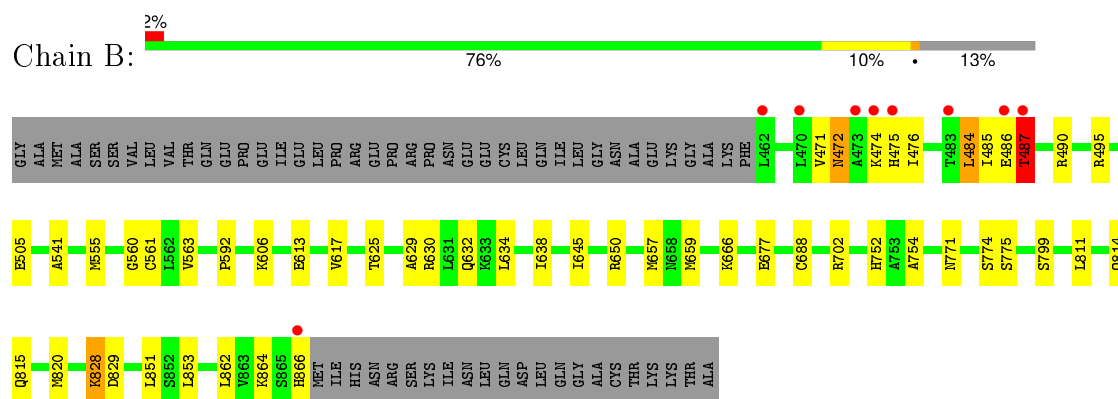
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

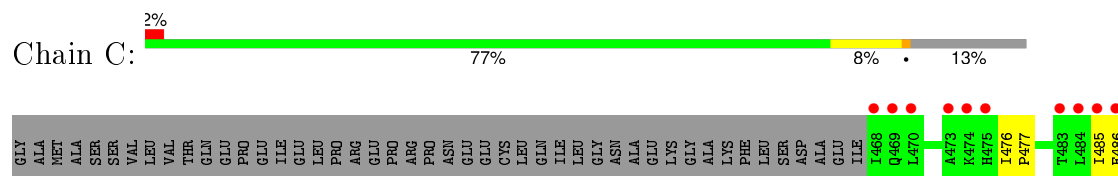
• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

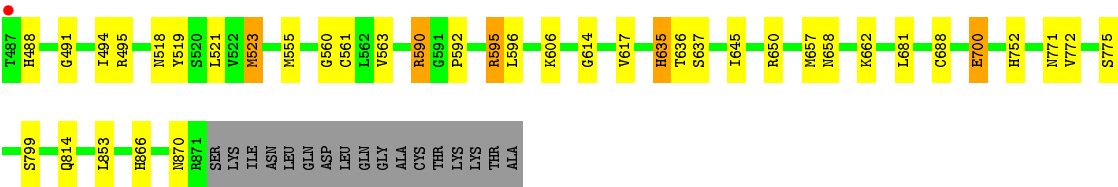


• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

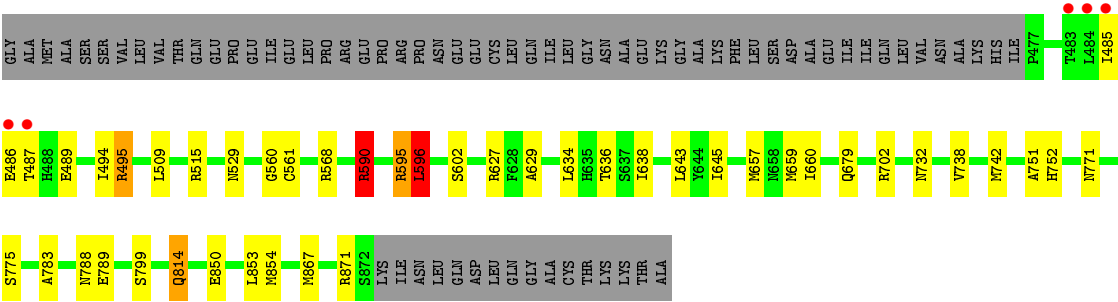


• Molecule 1: PROTEIN (HMG-COA REDUCTASE)





● Molecule 1: PROTEIN (HMG-COA REDUCTASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.92Å 172.63Å 73.99Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	44.00 – 2.00 38.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.00-2.00) 49.9 (38.37-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.65 (at 2.00Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.168 , 0.197 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.1	EDS
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.053 for h,-k,-h-l 0.069 for -h-l,-k,l 0.046 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54850 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12909	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: COA, MAH, 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	0.55	0/3089	0.72	1/4177 (0.0%)
1	B	0.54	0/3054	0.73	2/4130 (0.0%)
1	C	0.54	0/3056	0.74	4/4131 (0.1%)
1	D	0.57	0/2989	0.77	6/4039 (0.1%)
All	All	0.55	0/12188	0.74	13/16477 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	590	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	495	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	D	568	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	C	590	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	D	495	ARG	NE-CZ-NH2	-6.66	116.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	749	TYR	Sidechain

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	3044	0	3085	45	0
1	B	3010	0	3052	49	0
1	C	3011	0	3056	38	0
1	D	2945	0	2981	26	0
2	A	48	0	32	2	0
2	B	48	0	32	4	0
2	C	48	0	32	6	0
2	D	48	0	32	1	0
3	A	11	0	8	2	0
3	B	11	0	8	1	0
3	C	11	0	8	0	0
3	D	11	0	8	0	0
4	A	48	0	25	7	0
4	B	48	0	25	5	0
4	C	48	0	25	0	0
4	D	48	0	25	4	0
5	A	121	0	0	4	0
5	B	119	0	0	1	0
5	C	106	0	0	2	0
5	D	125	0	0	0	0
All	All	12909	0	12434	160	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 160 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:657:MET:HG2	4:A:1:NAP:C4N	1.93	0.99
1:B:657:MET:HG2	4:B:2:NAP:C4N	1.93	0.99
1:A:866:HIS:HE1	2:A:101:COA:HN4	1.19	0.86
1:B:625:THR:HG22	1:B:666:LYS:HD2	1.58	0.84
1:A:475:HIS:O	1:A:475:HIS:ND1	2.12	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/467 (87%)	391 (96%)	15 (4%)	1 (0%)	52	48
1	B	403/467 (86%)	381 (94%)	19 (5%)	3 (1%)	26	19
1	C	402/467 (86%)	388 (96%)	14 (4%)	0	100	100
1	D	394/467 (84%)	378 (96%)	16 (4%)	0	100	100
All	All	1606/1868 (86%)	1538 (96%)	64 (4%)	4 (0%)	52	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	HIS
1	B	484	LEU
1	B	864	LYS
1	B	487	THR

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	327/375 (87%)	314 (96%)	13 (4%)	38	33
1	B	323/375 (86%)	313 (97%)	10 (3%)	47	46
1	C	323/375 (86%)	315 (98%)	8 (2%)	55	55
1	D	316/375 (84%)	305 (96%)	11 (4%)	43	40
All	All	1289/1500 (86%)	1247 (97%)	42 (3%)	45	43

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	688	CYS
1	C	523	MET
1	D	752	HIS
1	B	752	HIS
1	B	828	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	475	HIS
1	B	632	GLN
1	C	861	HIS
1	B	472	ASN
1	C	635	HIS

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
4	NAP	A	1	-	42,52,52	1.75	8 (19%)	54,80,80	1.61	7 (12%)
2	COA	A	101	-	40,50,50	1.65	6 (15%)	50,75,75	1.38	8 (16%)
3	MAH	A	201	-	4,10,10	2.13	1 (25%)	2,14,14	0.92	0
2	COA	B	102	-	40,50,50	1.74	6 (15%)	50,75,75	1.43	8 (16%)
4	NAP	B	2	-	42,52,52	1.75	8 (19%)	54,80,80	1.58	7 (12%)
3	MAH	B	202	-	4,10,10	1.66	1 (25%)	2,14,14	0.75	0
2	COA	C	103	-	40,50,50	1.79	5 (12%)	50,75,75	1.41	7 (14%)
3	MAH	C	204	-	4,10,10	1.41	1 (25%)	2,14,14	0.90	0
4	NAP	C	3	-	42,52,52	1.67	2 (4%)	54,80,80	1.58	9 (16%)
2	COA	D	104	-	40,50,50	1.76	5 (12%)	50,75,75	1.58	9 (18%)
3	MAH	D	203	-	4,10,10	1.29	1 (25%)	2,14,14	0.69	0
4	NAP	D	4	-	42,52,52	1.79	6 (14%)	54,80,80	1.60	6 (11%)

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
4	NAP	A	1	-	-	0/27/67/67	0/5/5/5
2	COA	A	101	-	1/1/11/13	0/44/64/64	0/3/3/3
3	MAH	A	201	-	-	0/6/10/10	0/0/0/0
2	COA	B	102	-	1/1/11/13	0/44/64/64	0/3/3/3
4	NAP	B	2	-	-	0/27/67/67	0/5/5/5
3	MAH	B	202	-	-	0/6/10/10	0/0/0/0
2	COA	C	103	-	1/1/11/13	0/44/64/64	0/3/3/3
3	MAH	C	204	-	-	0/6/10/10	0/0/0/0
4	NAP	C	3	-	-	0/27/67/67	0/5/5/5
2	COA	D	104	-	1/1/11/13	0/44/64/64	0/3/3/3
3	MAH	D	203	-	-	0/6/10/10	0/0/0/0
4	NAP	D	4	-	-	0/27/67/67	0/5/5/5

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	NAP	P2B-O2X	2.02	1.62	1.54
4	A	1	NAP	PN-O1N	2.02	1.58	1.51
4	B	2	NAP	PN-O1N	2.09	1.58	1.51
4	A	1	NAP	O4D-C1D	2.09	1.43	1.41
4	D	4	NAP	C5A-C4A	2.14	1.45	1.40

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAP	O7N-C7N-N7N	-6.19	113.89	122.59
4	D	4	NAP	O7N-C7N-N7N	-6.18	113.89	122.59
4	A	1	NAP	O7N-C7N-N7N	-6.17	113.91	122.59
4	C	3	NAP	O7N-C7N-N7N	-6.01	114.14	122.59
4	A	1	NAP	PN-O3-PA	-4.46	120.20	132.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	101	COA	C3B
2	D	104	COA	C3B
2	C	103	COA	C3B
2	B	102	COA	C3B

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAP	7	0
2	A	101	COA	2	0
3	A	201	MAH	2	0
2	B	102	COA	4	0
4	B	2	NAP	5	0
3	B	202	MAH	1	0
2	C	103	COA	6	0
2	D	104	COA	1	0
4	D	4	NAP	4	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 [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	409/467 (87%)	-0.27	20 (4%) 33 35	8, 17, 45, 68	0
1	B	405/467 (86%)	-0.47	9 (2%) 65 66	9, 17, 42, 74	0
1	C	404/467 (86%)	-0.36	11 (2%) 58 58	8, 16, 43, 71	0
1	D	396/467 (84%)	-0.59	5 (1%) 79 80	8, 15, 32, 62	0
All	All	1614/1868 (86%)	-0.42	45 (2%) 56 57	8, 16, 42, 74	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	6.2
1	D	484	LEU	5.8
1	C	485	ILE	5.7
1	C	484	LEU	5.6
1	A	476	ILE	5.4

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(\AA^2)	Q<0.9
3	MAH	C	204	11/11	0.98	0.10	-0.02	12,13,16,17	0
4	NAP	B	2	48/48	0.96	0.09	-0.09	18,28,36,38	0
4	NAP	A	1	48/48	0.94	0.10	-0.26	23,32,40,41	0
4	NAP	D	4	48/48	0.98	0.07	-0.26	14,19,26,29	0
2	COA	D	104	48/48	0.97	0.08	-0.33	14,18,30,34	0
2	COA	C	103	48/48	0.96	0.08	-0.36	17,23,41,43	0
2	COA	A	101	48/48	0.98	0.07	-0.42	11,16,32,37	0
4	NAP	C	3	48/48	0.97	0.07	-0.50	14,18,22,26	0
3	MAH	D	203	11/11	0.98	0.08	-0.50	13,14,18,19	0
2	COA	B	102	48/48	0.96	0.08	-0.52	18,24,35,38	0
3	MAH	B	202	11/11	0.98	0.09	-0.72	16,18,21,23	0
3	MAH	A	201	11/11	0.98	0.07	-0.73	10,13,19,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.