



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:09 AM GMT

PDB ID : 3CD0
Title : Thermodynamic and structure guided design of statin hmg-coa reductase inhibitors
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Deposited on : 2008-02-26
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

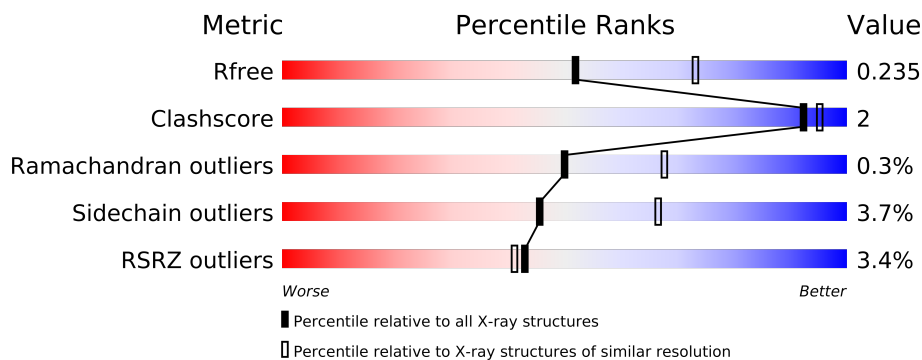
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	FAILED
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	441	
1	B	441	
1	C	441	
1	D	441	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13075 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-hydroxy-3-methylglutaryl-coenzymeA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3133	1951	551	601	30			
1	B	421	Total	C	N	O	S	0	1	0
			3136	1952	552	602	30			
1	C	414	Total	C	N	O	S	0	1	0
			3079	1918	541	590	30			
1	D	396	Total	C	N	O	S	0	0	0
			2934	1826	518	561	29			

There are 28 discrepancies between the modelled and reference sequences:

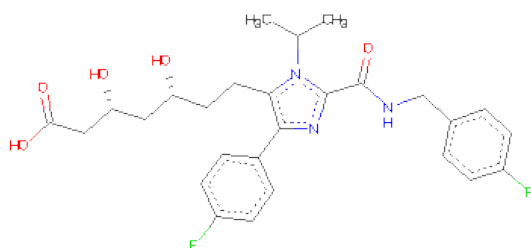
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered	UNP P04035
B	435	HIS	-	expression tag	UNP P04035
B	436	HIS	-	expression tag	UNP P04035
B	437	HIS	-	expression tag	UNP P04035
B	438	HIS	-	expression tag	UNP P04035
B	439	HIS	-	expression tag	UNP P04035
B	440	HIS	-	expression tag	UNP P04035
B	485	ILE	MET	engineered	UNP P04035
C	435	HIS	-	expression tag	UNP P04035
C	436	HIS	-	expression tag	UNP P04035
C	437	HIS	-	expression tag	UNP P04035
C	438	HIS	-	expression tag	UNP P04035
C	439	HIS	-	expression tag	UNP P04035
C	440	HIS	-	expression tag	UNP P04035
C	485	ILE	MET	engineered	UNP P04035

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Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered	UNP P04035

- Molecule 2 is (3R,5R)-7-{2-[(4-FLUOROBENZYL)CARBAMOYL]-4-(4-FLUOROPHENYL)-1-(1-METHYLETHYL)-1H-IMIDAZOL-5-YL}-3,5-DIHYDROXYHEPTANOICACID (three-letter code: 6HI) (formula: C₂₇H₃₁F₂N₃O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			37	27	2	3	5		
2	B	1	Total	C	F	N	O	0	0
			37	27	2	3	5		
2	C	1	Total	C	F	N	O	0	0
			37	27	2	3	5		
2	D	1	Total	C	F	N	O	0	0
			37	27	2	3	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total	O	0	0
			185	185		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	167	Total 167	O 167	0	0
3	C	118	Total 118	O 118	0	0
3	D	175	Total 175	O 175	0	0

4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.68Å 173.96Å 76.40Å 90.00° 119.06° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 43.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.40) 97.5 (43.78-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.238 0.193 , 0.235	Depositor DCC
R_{free} test set	3290 reflections (5.41%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13075	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6HI

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	0/3179	0.65	6/4298 (0.1%)
1	B	0.37	0/3187	0.64	5/4309 (0.1%)
1	C	0.36	0/3127	0.62	4/4225 (0.1%)
1	D	0.38	0/2975	0.64	3/4019 (0.1%)
All	All	0.37	0/12468	0.64	18/16851 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ASP	CB-CG-OD2	6.19	123.88	118.30
1	C	623	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	547	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	623	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	790	ASP	CB-CG-OD2	5.86	123.57	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3133	0	3167	14	0
1	B	3136	0	3169	12	0
1	C	3079	0	3119	9	0
1	D	2934	0	2967	11	0
2	B	74	0	60	2	0
2	C	37	0	30	1	0
2	D	37	0	30	2	0
3	A	185	0	0	0	0
3	B	167	0	0	1	0
3	C	118	0	0	1	0
3	D	175	0	0	1	0
All	All	13075	0	12542	46	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 46 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:771:ASN:OD1	1:C:775:SER:OG	2.18	0.61
2:B:2:6HI:H7A	2:B:2:6HI:H4A	1.83	0.59
2:C:4:6HI:H7A	2:C:4:6HI:H4A	1.84	0.57
1:B:752:HIS:HE1	1:B:849:GLY:C	2.09	0.56
1:D:595:ARG:HD2	1:D:681:LEU:HD22	1.87	0.56

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	419/441 (95%)	398 (95%)	17 (4%)	4 (1%)	22	32
1	B	420/441 (95%)	405 (96%)	15 (4%)	0	100	100
1	C	411/441 (93%)	398 (97%)	13 (3%)	0	100	100
1	D	392/441 (89%)	375 (96%)	16 (4%)	1 (0%)	50	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1642/1764 (93%)	1576 (96%)	61 (4%)	5 (0%)	50 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ALA
1	A	478	ALA
1	A	475	HIS
1	D	514	TYR
1	A	477	PRO

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	335/355 (94%)	320 (96%)	15 (4%)	38 57
1	B	336/355 (95%)	322 (96%)	14 (4%)	40 60
1	C	330/355 (93%)	319 (97%)	11 (3%)	50 71
1	D	313/355 (88%)	302 (96%)	11 (4%)	48 69
All	All	1314/1420 (92%)	1263 (96%)	51 (4%)	45 64

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	634	LEU
1	B	828	LYS
1	D	669	SER
1	B	669	SER
1	C	486	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	529	ASN
1	B	752	HIS

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Mol	Chain	Res	Type
1	D	518	ASN
1	B	472	ASN
1	D	472	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	6HI	B	1	-	39,39,39	0.93	1 (2%)	54,54,54	3.41	9 (16%)
2	6HI	B	2	-	39,39,39	0.90	1 (2%)	54,54,54	2.90	7 (12%)
2	6HI	C	4	-	39,39,39	0.87	1 (2%)	54,54,54	2.52	10 (18%)
2	6HI	D	3	-	39,39,39	0.85	1 (2%)	54,54,54	2.88	9 (16%)

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	6HI	B	1	-	-	0/26/30/30	0/3/3/3
2	6HI	B	2	-	-	0/26/30/30	0/3/3/3
2	6HI	C	4	-	-	0/26/30/30	0/3/3/3
2	6HI	D	3	-	-	0/26/30/30	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	6HI	C5-C12	3.86	1.49	1.40
2	B	1	6HI	C5-C12	3.65	1.49	1.40
2	C	4	6HI	C5-C12	3.47	1.48	1.40
2	D	3	6HI	C5-C12	3.28	1.48	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	6HI	C3-C2-N3	-22.01	120.98	124.59
2	B	2	6HI	C3-C2-N3	-17.76	121.68	124.59
2	D	3	6HI	C3-C2-N3	-16.55	121.88	124.59
2	C	4	6HI	C3-C2-N3	-12.68	122.51	124.59
2	D	3	6HI	C7-C12-N4	5.64	130.75	123.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	421/441 (95%)	-0.03	14 (3%) 44 42	22, 33, 63, 71	0
1	B	421/441 (95%)	-0.12	7 (1%) 67 65	22, 34, 46, 59	0
1	C	414/441 (93%)	0.06	19 (4%) 31 29	21, 38, 71, 94	1 (0%)
1	D	396/441 (89%)	-0.03	17 (4%) 34 32	21, 34, 70, 99	0
All	All	1652/1764 (93%)	-0.03	57 (3%) 43 40	21, 34, 62, 99	1 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	861	HIS	6.4
1	D	458	GLY	6.0
1	D	470	LEU	5.7
1	D	475	HIS	5.5
1	D	474	LYS	5.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	6HI	D	3	37/37	0.17	1.41	23,35,38,39	0
2	6HI	C	4	37/37	0.17	0.84	24,38,42,45	0
2	6HI	B	1	37/37	0.14	-0.09	26,33,39,41	0
2	6HI	B	2	37/37	0.14	-0.29	23,30,36,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.