



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:06 AM GMT

PDB ID : 3CDB  
Title : Thermodynamic and structure guided design of statin hmg-coa reductase inhibitors  
Authors : Pavlovsky, A.; Sarver, R.W.; Harris, M.S.; Finzel, B.C.  
Deposited on : 2008-02-26  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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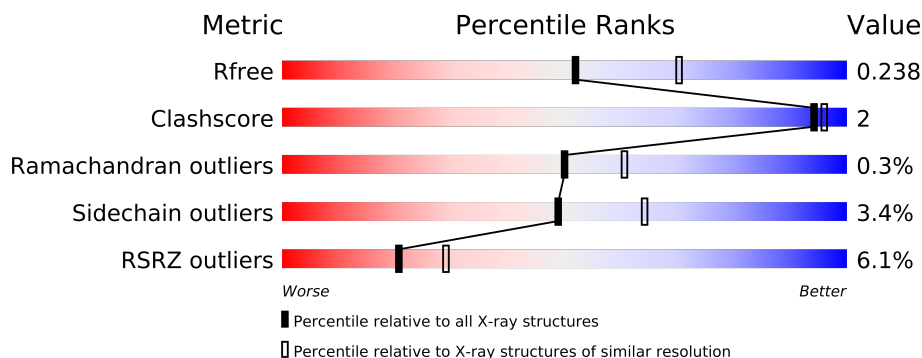
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. 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 13109 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	2	0
			3139	1954	552	602	31			
1	C	415	Total	C	N	O	S	0	1	0
			3086	1923	541	591	31			
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:

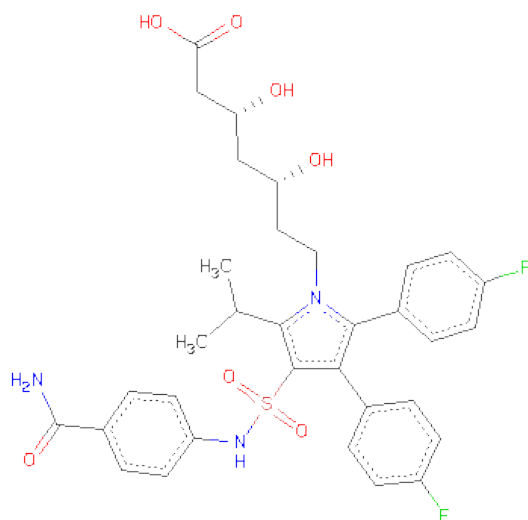
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered	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-{3-[4-CARBAMOYLPHENYL]SULFAMOYL}-4,5-BIS(4-FLUOROPHENYL)-2-(1-METHYLETHYL)-1H-PYRROL-1-YL}-3,5-DIHYDROXYHEPTANOIC ACID (three-letter code: 9HI) (formula: C<sub>33</sub>H<sub>35</sub>F<sub>2</sub>N<sub>3</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		
2	A	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		
2	C	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		
2	D	1	Total	C	F	N	O	S	0	0
			46	33	2	3	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total	O	0	0
			180	180		

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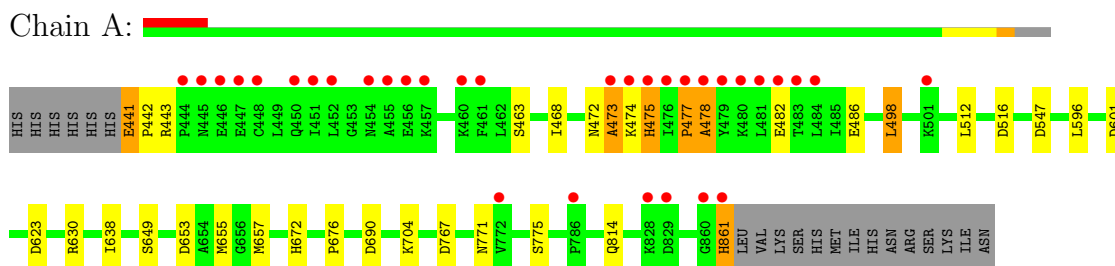
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	159	Total 159	O 159	0	0
3	C	122	Total 122	O 122	0	0
3	D	172	Total 172	O 172	0	0

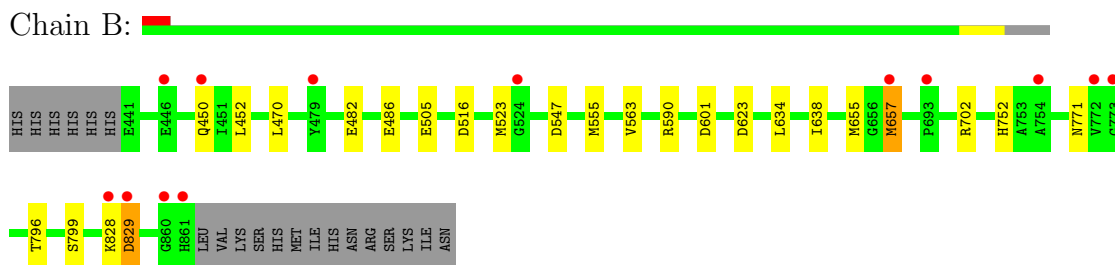
### 3 Residue-property plots

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.

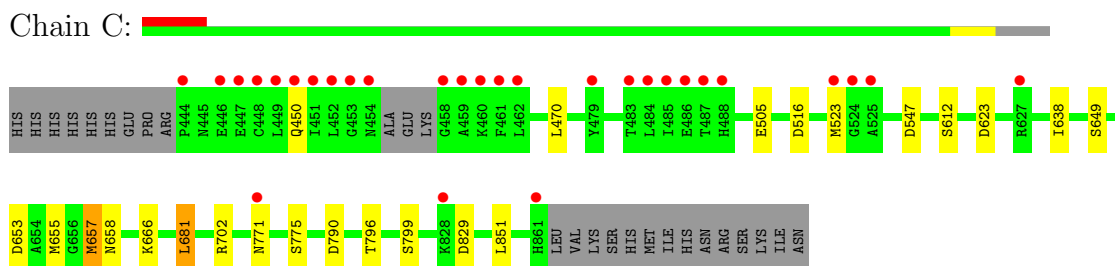
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase



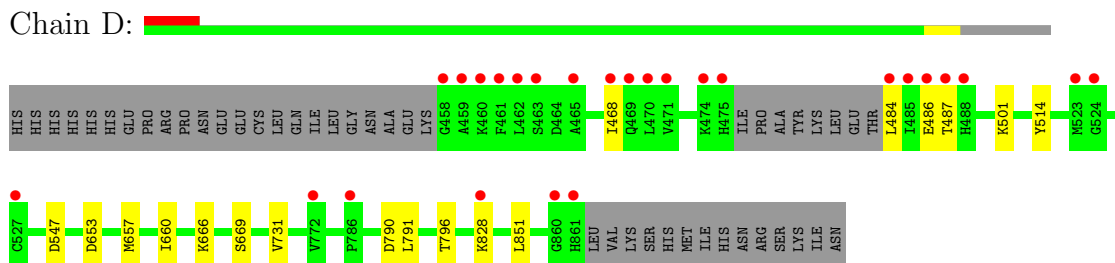
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase



## 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, $\alpha$ , $\beta$ , $\gamma$	73.58Å 173.48Å 75.99Å 90.00° 118.68° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 43.68 – 2.29	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-2.30) 92.4 (43.68-2.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.202 , 0.239 0.205 , 0.238	Depositor DCC
$R_{free}$ test set	3509 reflections (5.37%)	DCC
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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: 9HI

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	0.33	0/3179	0.62	6/4298 (0.1%)
1	B	0.33	0/3195	0.62	5/4319 (0.1%)
1	C	0.32	0/3135	0.60	6/4236 (0.1%)
1	D	0.33	0/2975	0.61	3/4019 (0.1%)
All	All	0.33	0/12484	0.61	20/16872 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	623	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	623	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	547	ASP	CB-CG-OD2	5.74	123.46	118.30
1	C	547	ASP	CB-CG-OD2	5.72	123.45	118.30
1	D	547	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	516	ASP	CB-CG-OD2	5.70	123.42	118.30
1	A	516	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	547	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	790	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	653	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	790	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	516	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	829	ASP	CB-CG-OD2	5.34	123.10	118.30
1	C	653	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	623	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	601	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	829	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	653	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	767	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	690	ASP	CB-CG-OD2	5.02	122.82	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	13	0
1	B	3139	0	3174	6	0
1	C	3086	0	3122	7	0
1	D	2934	0	2967	3	0
2	A	92	0	68	8	0
2	C	46	0	34	3	0
2	D	46	0	34	3	0
3	A	180	0	0	0	0
3	B	159	0	0	1	0
3	C	122	0	0	0	0
3	D	172	0	0	0	0
All	All	13109	0	12566	38	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.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:2:9HI:H7	2:A:2:9HI:H13B	1.71	0.70
1:A:655:MET:SD	1:A:657:MET:HG3	2.32	0.69
2:D:3:9HI:H7	2:D:3:9HI:H13B	1.76	0.67
2:A:1:9HI:H7	2:A:1:9HI:H13B	1.77	0.66
2:C:4:9HI:H7	2:C:4:9HI:H13B	1.79	0.64
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.79	0.64
1:C:771:ASN:OD1	1:C:775:SER:OG	2.15	0.63
2:A:1:9HI:H26	2:A:1:9HI:C2	2.31	0.60
2:A:1:9HI:C12	2:A:1:9HI:H26	2.32	0.59
1:A:861:HIS:HA	2:A:1:9HI:F2	1.96	0.55
2:D:3:9HI:H8A	2:D:3:9HI:H14B	1.93	0.51
2:C:4:9HI:H6	2:C:4:9HI:O1	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:655:MET:SD	1:B:657[B]:MET:HG3	2.51	0.51
1:A:441:GLU:N	1:A:442:PRO:CD	2.73	0.50
2:D:3:9HI:O1	2:D:3:9HI:H6	2.12	0.50
1:A:472:ASN:O	1:A:473:ALA:HB3	2.13	0.49
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.94	0.49
2:A:2:9HI:O1	2:A:2:9HI:H6	2.14	0.48
1:C:657[B]:MET:HG3	1:C:658:ASN:N	2.28	0.48
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.48	0.48
1:A:472:ASN:O	1:A:473:ALA:CB	2.62	0.48
1:A:638:ILE:O	1:D:796:THR:HG21	2.13	0.48
1:B:638:ILE:O	1:C:796:THR:HG21	2.14	0.47
1:A:474:LYS:O	1:A:475:HIS:HB2	2.15	0.46
1:A:477:PRO:O	1:A:478:ALA:HB2	2.17	0.45
1:B:590:ARG:HD2	3:B:984:HOH:O	2.17	0.45
1:A:596:LEU:HB3	1:A:601:ASP:HB2	1.99	0.45
1:B:702:ARG:O	1:B:799:SER:HA	2.17	0.45
1:A:468:ILE:HG12	1:A:498:LEU:CD1	2.48	0.44
1:C:702:ARG:O	1:C:799:SER:HA	2.17	0.43
1:A:771:ASN:OD1	1:A:775:SER:OG	2.36	0.43
1:B:796:THR:HG21	1:C:638:ILE:O	2.19	0.42
2:A:1:9HI:H8A	2:A:1:9HI:H14B	2.01	0.42
1:A:474:LYS:O	1:A:475:HIS:CB	2.67	0.42
2:C:4:9HI:H14B	2:C:4:9HI:H8A	2.02	0.41
1:D:468:ILE:HG21	1:D:501:LYS:NZ	2.36	0.41
2:A:1:9HI:C26	2:A:1:9HI:C2	2.99	0.41
1:C:655:MET:SD	1:C:657[A]:MET:HG3	2.61	0.41

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%)	395 (94%)	20 (5%)	4 (1%)	22	23
1	B	421/441 (96%)	409 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	412/441 (93%)	396 (96%)	16 (4%)	0	100	100
1	D	392/441 (89%)	378 (96%)	13 (3%)	1 (0%)	50	60
All	All	1644/1764 (93%)	1578 (96%)	61 (4%)	5 (0%)	50	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ALA
1	A	475	HIS
1	A	478	ALA
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%)	323 (96%)	12 (4%)	47	61
1	B	337/355 (95%)	322 (96%)	15 (4%)	38	50
1	C	331/355 (93%)	320 (97%)	11 (3%)	50	66
1	D	313/355 (88%)	303 (97%)	10 (3%)	51	67
All	All	1316/1420 (93%)	1268 (96%)	48 (4%)	49	61

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	443	ARG
1	A	463	SER
1	A	482	GLU
1	A	486	GLU
1	A	498	LEU
1	A	512	LEU
1	A	630	ARG
1	A	649	SER

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Mol	Chain	Res	Type
1	A	704	LYS
1	A	814	GLN
1	A	861	HIS
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	482	GLU
1	B	486	GLU
1	B	505	GLU
1	B	523	MET
1	B	634	LEU
1	B	657[A]	MET
1	B	657[B]	MET
1	B	752	HIS
1	B	771[A]	ASN
1	B	771[B]	ASN
1	B	828	LYS
1	B	829	ASP
1	C	450	GLN
1	C	470	LEU
1	C	505	GLU
1	C	523	MET
1	C	612	SER
1	C	649	SER
1	C	657[A]	MET
1	C	657[B]	MET
1	C	666	LYS
1	C	681	LEU
1	C	851	LEU
1	D	484	LEU
1	D	486	GLU
1	D	487	THR
1	D	657	MET
1	D	660	ILE
1	D	666	LYS
1	D	669	SER
1	D	791	LEU
1	D	828	LYS
1	D	851	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	ASN
1	A	510	GLN
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN
1	A	819	GLN
1	B	450	GLN
1	B	472	ASN
1	B	529	ASN
1	C	469	GLN
1	C	472	ASN
1	C	679	GLN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	861	HIS

### 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	9HI	A	1	-	49,49,49	1.48	4 (8%)	68,71,71	2.16	12 (17%)
2	9HI	A	2	-	49,49,49	1.49	4 (8%)	68,71,71	2.15	16 (23%)
2	9HI	C	4	-	49,49,49	1.54	4 (8%)	68,71,71	2.04	13 (19%)
2	9HI	D	3	-	49,49,49	1.48	4 (8%)	68,71,71	1.91	12 (17%)

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	9HI	A	1	-	-	0/34/40/40	0/4/4/4
2	9HI	A	2	-	-	0/34/40/40	0/4/4/4
2	9HI	C	4	-	-	0/34/40/40	0/4/4/4
2	9HI	D	3	-	-	0/34/40/40	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	9HI	C2-S1	-7.30	1.65	1.79
2	A	1	9HI	C2-S1	-7.10	1.65	1.79
2	A	2	9HI	C2-S1	-7.06	1.66	1.79
2	D	3	9HI	C2-S1	-6.86	1.66	1.79
2	A	1	9HI	C5-N1	-4.48	1.34	1.40
2	C	4	9HI	C5-N1	-4.29	1.35	1.40
2	D	3	9HI	C5-N1	-4.11	1.35	1.40
2	A	2	9HI	C5-N1	-4.01	1.35	1.40
2	C	4	9HI	C32-N2	-3.92	1.36	1.42
2	D	3	9HI	C32-N2	-3.90	1.36	1.42
2	A	2	9HI	C32-N2	-3.69	1.37	1.42
2	A	1	9HI	C32-N2	-3.37	1.37	1.42
2	D	3	9HI	C1-C5	3.05	1.46	1.41
2	A	2	9HI	C1-C5	2.91	1.46	1.41
2	C	4	9HI	C1-C5	2.75	1.46	1.41
2	A	1	9HI	C1-C5	2.53	1.45	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	9HI	O2-S1-O1	-9.99	106.11	119.55
2	D	3	9HI	O2-S1-O1	-8.59	108.00	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	9HI	O2-S1-O1	-8.57	108.03	119.55
2	C	4	9HI	O2-S1-O1	-8.47	108.15	119.55
2	C	4	9HI	C27-C5-N1	7.52	135.96	122.27
2	A	1	9HI	C27-C5-N1	7.30	135.56	122.27
2	D	3	9HI	C27-C5-N1	6.46	134.03	122.27
2	A	2	9HI	C27-C5-N1	6.15	133.46	122.27
2	C	4	9HI	C1-C5-C27	-6.05	116.56	129.13
2	A	2	9HI	C7-C8-C9	-5.81	108.30	113.82
2	A	1	9HI	C1-C5-C27	-5.80	117.06	129.13
2	D	3	9HI	C1-C5-C27	-5.40	117.91	129.13
2	A	2	9HI	C1-C5-C27	-4.99	118.76	129.13
2	C	4	9HI	C7-C8-C9	-4.62	109.43	113.82
2	A	2	9HI	C8-C7-N1	3.89	115.48	112.31
2	A	1	9HI	C7-C8-C9	-3.50	110.50	113.82
2	A	1	9HI	C2-S1-N2	3.38	112.44	107.31
2	A	1	9HI	C8-C7-N1	-3.18	109.72	112.31
2	A	2	9HI	O1-S1-C2	3.07	113.35	108.87
2	A	2	9HI	C11-C10-C9	-2.95	110.47	114.65
2	A	2	9HI	C1-C2-C12	2.84	109.83	107.51
2	D	3	9HI	C19-C28-C22	-2.69	119.25	122.90
2	D	3	9HI	C1-C2-C12	2.62	109.65	107.51
2	D	3	9HI	C25-C22-C28	2.58	121.06	118.33
2	A	2	9HI	C31-C1-C2	2.54	129.67	127.07
2	A	1	9HI	O1-S1-C2	2.52	112.55	108.87
2	D	3	9HI	C7-C8-C9	-2.51	111.44	113.82
2	C	4	9HI	C31-C1-C2	2.50	129.63	127.07
2	A	2	9HI	C7-N1-C5	-2.50	120.87	124.83
2	A	2	9HI	C7-N1-C12	2.45	128.82	124.72
2	C	4	9HI	C1-C2-C12	2.37	109.44	107.51
2	A	2	9HI	C2-C12-C6	-2.34	125.70	131.15
2	C	4	9HI	C11-C10-C9	-2.31	111.38	114.65
2	D	3	9HI	O1-S1-C2	2.30	112.22	108.87
2	A	1	9HI	C1-C2-C12	2.30	109.39	107.51
2	A	1	9HI	C2-C12-C6	-2.27	125.87	131.15
2	C	4	9HI	C19-C28-C22	-2.24	119.85	122.90
2	A	2	9HI	C25-C22-C28	2.24	120.70	118.33
2	C	4	9HI	O1-S1-C2	2.20	112.08	108.87
2	A	1	9HI	C25-C31-C1	-2.19	117.11	120.77
2	A	1	9HI	C10-C11-C35	-2.18	108.45	113.02
2	D	3	9HI	C2-C12-C6	-2.14	126.16	131.15
2	A	2	9HI	C19-C28-C22	-2.14	119.99	122.90
2	D	3	9HI	C7-N1-C12	2.10	128.25	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	9HI	C26-C32-N2	2.10	124.73	120.07
2	C	4	9HI	C2-C12-C6	-2.07	126.32	131.15
2	A	1	9HI	C5-N1-C12	2.07	110.27	108.81
2	C	4	9HI	C10-C11-C35	-2.06	108.71	113.02
2	D	3	9HI	C10-C11-C35	-2.04	108.75	113.02
2	C	4	9HI	C25-C22-C28	2.03	120.48	118.33
2	C	4	9HI	C24-C30-C15	-2.03	120.14	122.90
2	D	3	9HI	C24-C30-C15	-2.01	120.16	122.90
2	A	2	9HI	C14-C6-C12	-2.01	108.31	111.97

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, 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	421/441 (95%)	0.32	33 (7%) 13 19	20, 32, 58, 65	0
1	B	421/441 (95%)	0.09	13 (3%) 47 56	21, 32, 44, 53	0
1	C	415/441 (94%)	0.35	29 (6%) 16 23	19, 34, 69, 91	0
1	D	396/441 (89%)	0.23	26 (6%) 18 26	20, 31, 68, 95	0
All	All	1653/1764 (93%)	0.25	101 (6%) 21 29	19, 32, 58, 95	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	861	HIS	10.4
1	A	479	TYR	7.4
1	D	861	HIS	7.2
1	C	461	PHE	7.2
1	D	461	PHE	7.1
1	D	475	HIS	7.0
1	B	861	HIS	6.9
1	C	452	LEU	6.8
1	A	456	GLU	6.1
1	D	474	LYS	6.0
1	C	462	LEU	5.9
1	A	483	THR	5.9
1	A	477	PRO	5.7
1	D	458	GLY	5.6
1	D	486	GLU	5.4
1	C	460	LYS	5.3
1	C	450	GLN	5.2
1	C	451	ILE	5.2
1	A	452	LEU	4.9
1	A	480	LYS	4.9
1	B	860	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	483	THR	4.8
1	C	444	PRO	4.7
1	C	524	GLY	4.6
1	A	475	HIS	4.5
1	A	451	ILE	4.5
1	C	525	ALA	4.5
1	A	450	GLN	4.4
1	C	459	ALA	4.4
1	C	454	ASN	4.2
1	C	861	HIS	4.1
1	D	485	ILE	4.1
1	A	476	ILE	4.1
1	D	463	SER	4.0
1	D	470	LEU	3.9
1	D	860	GLY	3.8
1	B	524	GLY	3.7
1	D	484	LEU	3.7
1	A	482	GLU	3.7
1	A	444	PRO	3.7
1	D	460	LYS	3.6
1	B	657[A]	MET	3.5
1	D	468	ILE	3.5
1	A	484	LEU	3.4
1	D	469	GLN	3.3
1	A	478	ALA	3.3
1	C	487	THR	3.3
1	A	461	PHE	3.3
1	C	446	GLU	3.2
1	C	523	MET	3.2
1	A	473	ALA	3.2
1	A	447	GLU	3.2
1	D	471	VAL	3.1
1	A	829	ASP	3.1
1	B	446	GLU	3.0
1	C	458	GLY	3.0
1	D	465	ALA	3.0
1	A	457	LYS	3.0
1	A	772	VAL	3.0
1	B	829	ASP	2.9
1	A	455	ALA	2.9
1	C	486	GLU	2.9
1	A	474	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	459	ALA	2.9
1	C	484	LEU	2.8
1	C	447	GLU	2.7
1	A	446	GLU	2.7
1	A	448	CYS	2.7
1	C	771	ASN	2.7
1	B	479	TYR	2.7
1	D	523	MET	2.7
1	B	450	GLN	2.6
1	A	454	ASN	2.6
1	C	449	LEU	2.6
1	D	462	LEU	2.5
1	D	786	PRO	2.5
1	A	445	ASN	2.5
1	D	487	THR	2.4
1	D	524	GLY	2.4
1	C	453	GLY	2.3
1	A	481	LEU	2.3
1	D	488	HIS	2.3
1	C	485	ILE	2.3
1	C	828	LYS	2.3
1	D	828	LYS	2.3
1	A	460	LYS	2.2
1	C	627	ARG	2.2
1	B	773	GLY	2.2
1	B	693	PRO	2.1
1	A	786	PRO	2.1
1	B	772	VAL	2.1
1	A	860	GLY	2.1
1	A	828	LYS	2.1
1	B	828	LYS	2.1
1	D	527	CYS	2.1
1	D	772	VAL	2.1
1	A	501	LYS	2.1
1	B	754	ALA	2.1
1	C	488	HIS	2.0
1	C	479	TYR	2.0
1	C	448	CYS	2.0

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	9HI	D	3	46/46	0.18	0.63	25,44,52,54	0
2	9HI	C	4	46/46	0.19	0.26	29,45,53,53	0
2	9HI	A	1	46/46	0.19	0.11	27,44,53,55	0
2	9HI	A	2	46/46	0.17	0.08	29,44,50,52	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.