



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 AM GMT

PDB ID : 3CD0  
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 : 2.40 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](mailto: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

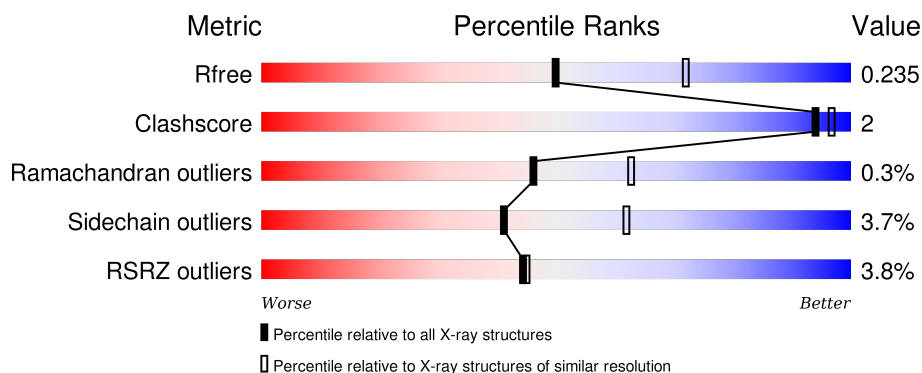
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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  $\geq 3$ , 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	441	<div> <div>3%</div> <div>87% 7% 5%</div> </div>
1	B	441	<div> <div>2%</div> <div>88% 7% 5%</div> </div>
1	C	441	<div> <div>5%</div> <div>88% 6% 6%</div> </div>
1	D	441	<div> <div>4%</div> <div>83% 7% 10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13075 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 3-hydroxy-3-methylglutaryl-coenzyme A 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:

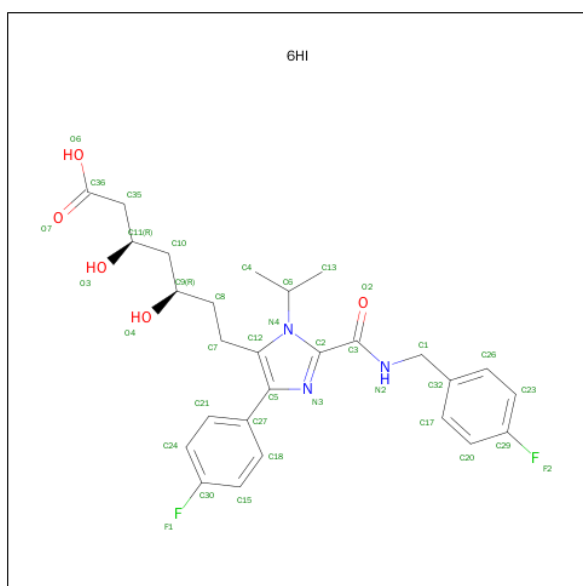
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered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

*Continued on next page...*

Continued from previous page...

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-DIHYDROXYHEPTANOIC ACID (three-letter code: 6HI) (formula: C<sub>27</sub>H<sub>31</sub>F<sub>2</sub>N<sub>3</sub>O<sub>5</sub>).



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		

Continued on next page...

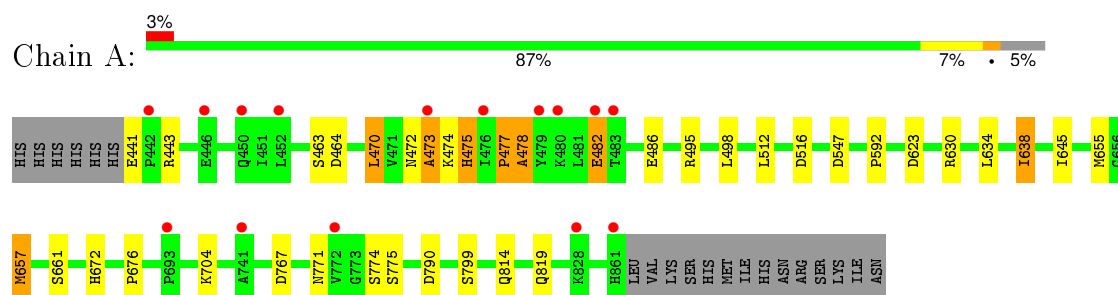
*Continued from previous page...*

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

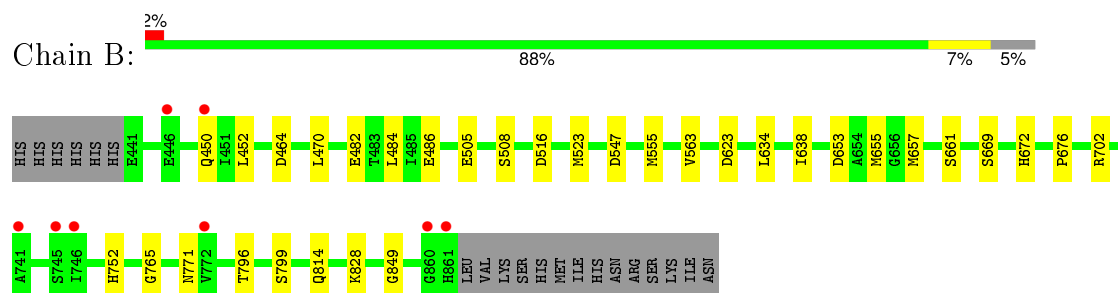
### 3 Residue-property plots

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.

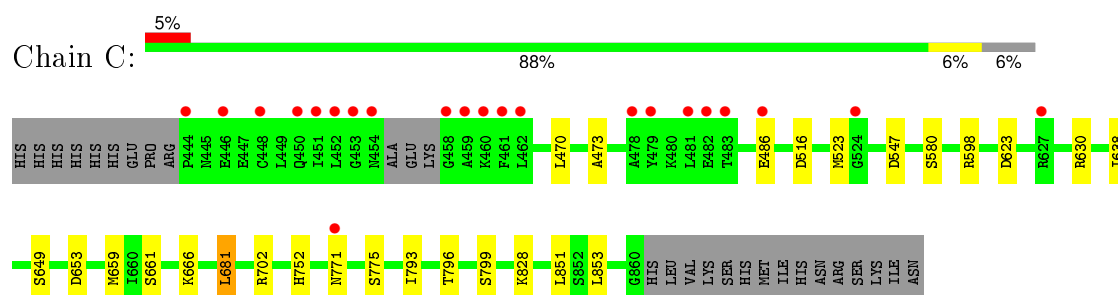
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



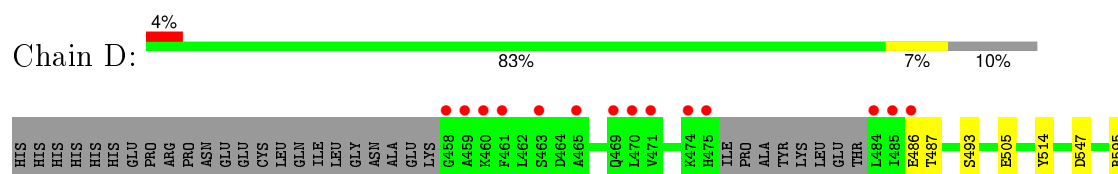
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

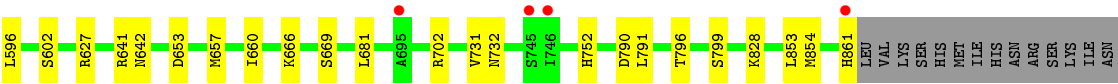


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 97.4 (43.78-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190 , 0.238 0.192 , 0.235	Depositor DCC
$R_{free}$ test set	3290 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.6	EDS
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.021 for h,-k,-h-l 0.020 for l,-k,h 0.020 for -h-l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 64107 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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: 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.

All (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
1	B	516	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	547	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	547	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	547	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	653	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	516	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	790	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	516	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	464	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	464	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	653	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	653	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	767	ASP	CB-CG-OD2	5.01	122.81	118.30

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	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

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 2.

All (46) 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: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
1:A:655:MET:SD	1:A:657:MET:HG3	2.47	0.55
1:D:657:MET:HG3	3:D:929:HOH:O	2.05	0.55
2:B:1:6HI:H7A	2:B:1:6HI:H4A	1.88	0.55
2:D:3:6HI:H7A	2:D:3:6HI:H4A	1.89	0.54
1:A:470:LEU:O	1:A:474:LYS:O	2.25	0.53
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.89	0.53
1:B:796:THR:HG21	1:C:638:ILE:O	2.09	0.53
1:B:655:MET:SD	1:B:657:MET:HG2	2.51	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:O	1:A:475:HIS:HB2	2.13	0.48
1:A:472:ASN:O	1:A:473:ALA:CB	2.61	0.47
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.49	0.47
1:B:638:ILE:O	1:C:796:THR:HG21	2.14	0.47
1:A:477:PRO:O	1:A:478:ALA:HB2	2.14	0.47
1:A:472:ASN:O	1:A:473:ALA:HB3	2.15	0.47
1:B:752:HIS:CE1	3:B:884:HOH:O	2.67	0.47
1:B:752:HIS:CG	1:B:752:HIS:O	2.68	0.46
2:D:3:6HI:H13B	2:D:3:6HI:H8A	1.96	0.46
1:D:702:ARG:O	1:D:799:SER:HA	2.15	0.46
1:C:793:ILE:HD13	1:C:851:LEU:HG	1.98	0.46
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.98	0.46
1:A:474:LYS:O	1:A:475:HIS:CB	2.64	0.45
1:A:638:ILE:O	1:D:796:THR:HG21	2.17	0.45
1:A:819:GLN:HB3	1:B:508:SER:HB3	1.98	0.45
1:A:774:SER:HA	1:A:799:SER:O	2.17	0.45
1:B:752:HIS:HE1	1:B:849:GLY:O	2.01	0.44
1:D:595:ARG:HE	1:D:642:ASN:ND2	2.16	0.43
1:D:595:ARG:HE	1:D:642:ASN:HD21	1.66	0.43
1:D:596:LEU:HD13	1:D:602:SER:HA	2.01	0.43
1:C:752:HIS:CD2	1:C:853:LEU:HD23	2.55	0.42
1:C:702:ARG:O	1:C:799:SER:HA	2.18	0.42
1:D:732:ASN:HA	1:D:854:MET:HE1	2.02	0.42
1:C:470:LEU:O	1:C:473:ALA:O	2.38	0.42
1:B:672:HIS:CE1	1:B:676:PRO:HA	2.55	0.42
1:D:596:LEU:O	1:D:641:ARG:HB2	2.19	0.41
1:A:592:PRO:HD2	1:A:645:ILE:O	2.20	0.41
1:D:752:HIS:CD2	1:D:853:LEU:HD23	2.56	0.41
1:A:771:ASN:OD1	1:A:775:SER:OG	2.39	0.41
1:B:702:ARG:O	1:B:799:SER:HA	2.20	0.41
1:C:661:SER:HB3	3:C:988:HOH:O	2.19	0.41
1:A:482:GLU:OE2	1:A:495:ARG:NH2	2.55	0.40
1:B:765:GLY:CA	1:B:814:GLN:HG2	2.52	0.40

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%)	19	28
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%)	46	63
All	All	1642/1764 (93%)	1576 (96%)	61 (4%)	5 (0%)	46	63

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%)	34	52
1	B	336/355 (95%)	322 (96%)	14 (4%)	36	56
1	C	330/355 (93%)	319 (97%)	11 (3%)	45	66
1	D	313/355 (88%)	302 (96%)	11 (4%)	43	64
All	All	1314/1420 (92%)	1263 (96%)	51 (4%)	41	59

All (51) 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	470	LEU
1	A	482	GLU
1	A	486	GLU
1	A	498	LEU
1	A	512	LEU
1	A	630	ARG
1	A	634	LEU
1	A	638	ILE
1	A	657	MET
1	A	661	SER
1	A	704	LYS
1	A	814	GLN
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	482	GLU
1	B	484	LEU
1	B	486	GLU
1	B	505	GLU
1	B	523	MET
1	B	634	LEU
1	B	661	SER
1	B	669	SER
1	B	771[A]	ASN
1	B	771[B]	ASN
1	B	828	LYS
1	C	486	GLU
1	C	523	MET
1	C	580	SER
1	C	598	ARG
1	C	630[A]	ARG
1	C	630[B]	ARG
1	C	649	SER
1	C	659	MET
1	C	666	LYS
1	C	681	LEU
1	C	828	LYS
1	D	486	GLU
1	D	487	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	493	SER
1	D	505	GLU
1	D	627	ARG
1	D	660	ILE
1	D	666	LYS
1	D	669	SER
1	D	791	LEU
1	D	828	LYS
1	D	861	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	567	ASN
1	A	632	GLN
1	A	861	HIS
1	B	450	GLN
1	B	472	ASN
1	B	529	ASN
1	B	752	HIS
1	C	469	GLN
1	C	472	ASN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	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

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	-	32,39,39	1.74	1 (3%)	39,54,54	1.33	4 (10%)
2	6HI	B	2	-	32,39,39	1.79	1 (3%)	39,54,54	1.27	3 (7%)
2	6HI	C	4	-	32,39,39	1.57	1 (3%)	39,54,54	1.31	5 (12%)
2	6HI	D	3	-	32,39,39	1.64	1 (3%)	39,54,54	1.30	4 (10%)

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	-	-	0/24/30/30	0/3/3/3
2	6HI	B	2	-	-	0/24/30/30	0/3/3/3
2	6HI	C	4	-	-	0/24/30/30	0/3/3/3
2	6HI	D	3	-	-	0/24/30/30	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	C2-C3	-9.40	1.49	1.53
2	B	1	6HI	C2-C3	-8.91	1.49	1.53
2	D	3	6HI	C2-C3	-8.26	1.49	1.53
2	C	4	6HI	C2-C3	-8.00	1.49	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	6HI	O2-C3-C2	-3.28	116.58	121.01
2	B	2	6HI	C5-C12-N4	-3.12	103.03	107.08
2	B	1	6HI	C5-C12-N4	-3.07	103.09	107.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	6HI	C5-C12-N4	-2.95	103.25	107.08
2	D	3	6HI	C5-C12-N4	-2.85	103.38	107.08
2	D	3	6HI	C7-C12-C5	-2.73	125.87	130.59
2	C	4	6HI	O2-C3-C2	-2.66	117.41	121.01
2	C	4	6HI	C7-C12-C5	-2.48	126.31	130.59
2	B	2	6HI	C10-C9-C8	-2.22	108.45	112.26
2	D	3	6HI	C10-C11-C35	-2.18	108.77	112.94
2	B	1	6HI	C23-C29-C20	-2.18	119.73	122.87
2	B	1	6HI	C24-C30-C15	-2.17	119.74	122.87
2	B	2	6HI	O2-C3-C2	-2.17	118.08	121.01
2	C	4	6HI	C10-C11-C35	-2.15	108.83	112.94
2	B	1	6HI	C4-C6-N4	-2.07	108.95	111.55
2	C	4	6HI	C13-C6-N4	-2.07	108.96	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	6HI	1	0
2	B	2	6HI	1	0
2	C	4	6HI	1	0
2	D	3	6HI	2	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 ⓘ

### 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%)	-0.05	15 (3%) 46 47	22, 33, 63, 71	0
1	B	421/441 (95%)	-0.15	8 (1%) 70 69	22, 34, 46, 59	0
1	C	414/441 (93%)	0.09	22 (5%) 30 30	21, 38, 71, 94	1 (0%)
1	D	396/441 (89%)	-0.06	18 (4%) 37 38	21, 34, 70, 99	0
All	All	1652/1764 (93%)	-0.05	63 (3%) 44 45	21, 34, 62, 99	1 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	861	HIS	7.4
1	D	458	GLY	6.8
1	D	475	HIS	6.0
1	C	452	LEU	5.9
1	D	470	LEU	5.7
1	D	474	LYS	5.4
1	D	461	PHE	5.3
1	C	451	ILE	5.3
1	C	461	PHE	5.0
1	A	479	TYR	4.9
1	C	453	GLY	4.3
1	B	861	HIS	4.2
1	A	452	LEU	4.1
1	C	460	LYS	4.1
1	D	459	ALA	4.1
1	C	483	THR	4.0
1	C	450	GLN	4.0
1	A	861	HIS	3.7
1	D	486	GLU	3.7
1	C	524	GLY	3.5
1	C	458	GLY	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	481	LEU	3.3
1	D	484	LEU	3.3
1	A	483	THR	3.3
1	A	450	GLN	3.3
1	A	482	GLU	3.2
1	D	463	SER	3.2
1	A	480	LYS	3.1
1	D	460	LYS	3.0
1	D	471	VAL	2.9
1	A	446	GLU	2.9
1	C	459	ALA	2.8
1	C	482	GLU	2.7
1	C	627	ARG	2.7
1	C	478	ALA	2.7
1	C	454	ASN	2.6
1	A	693	PRO	2.5
1	D	485	ILE	2.5
1	B	746	ILE	2.5
1	A	741	ALA	2.4
1	A	476	ILE	2.4
1	C	486	GLU	2.4
1	B	772	VAL	2.4
1	D	746	ILE	2.4
1	A	772	VAL	2.3
1	B	450	GLN	2.3
1	C	479	TYR	2.3
1	C	444	PRO	2.3
1	D	469	GLN	2.3
1	B	446	GLU	2.2
1	C	448	CYS	2.2
1	A	473	ALA	2.2
1	B	745	SER	2.2
1	D	745	SER	2.2
1	D	695	ALA	2.2
1	A	828	LYS	2.1
1	D	465	ALA	2.1
1	C	771	ASN	2.1
1	A	442	PRO	2.1
1	C	446	GLU	2.1
1	B	741	ALA	2.1
1	C	462	LEU	2.1
1	B	860	GLY	2.1

## 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	6HI	D	3	37/37	0.90	0.17	1.18	23,35,38,39	0
2	6HI	C	4	37/37	0.86	0.17	0.73	24,38,42,45	0
2	6HI	B	1	37/37	0.90	0.15	-0.06	26,33,39,41	0
2	6HI	B	2	37/37	0.93	0.14	-0.34	23,30,36,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.