



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:51 AM GMT

PDB ID : 3CCW  
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 : 2.10 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.

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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 : 1.7 (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

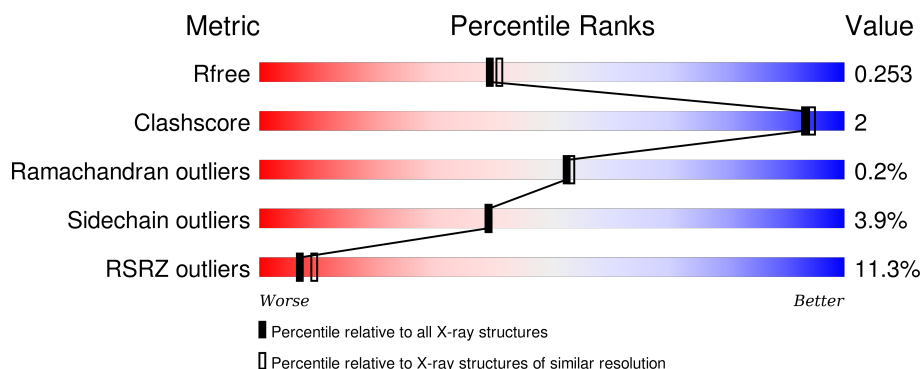
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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>15%</div> <div>87%</div> <div>7% • 5%</div> </div>
1	B	441	<div> <div>7%</div> <div>86%</div> <div>9% 5%</div> </div>
1	C	441	<div> <div>10%</div> <div>88%</div> <div>5% 6%</div> </div>
1	D	441	<div> <div>10%</div> <div>83%</div> <div>6% 11%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12823 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	0	0
			3133	1951	551	601	30			
1	C	414	Total	C	N	O	S	0	0	0
			3073	1915	538	590	30			
1	D	394	Total	C	N	O	S	0	0	0
			2920	1818	514	559	29			

There are 28 discrepancies between the modelled and reference sequences:

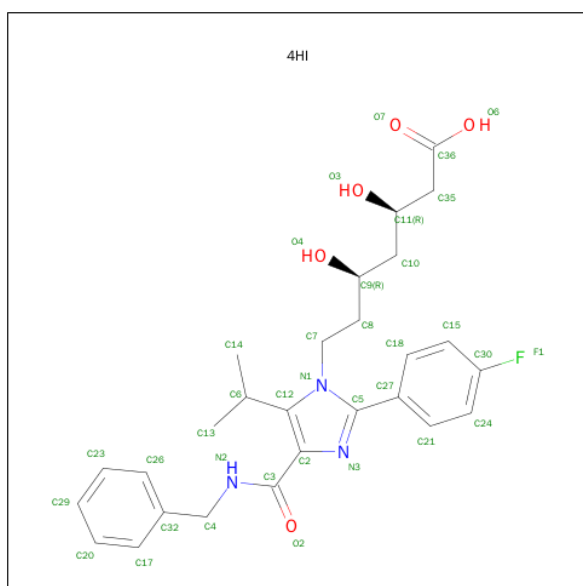
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered	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-[4-(BENZYL CARBAMOYL)-2-(4-FLUOROPHENYL)-5-(1-METHYLETHYL)-1H-IMIDAZOL-1-YL]-3,5-DIHYDROXYHEPTANOIC ACID (three-letter code: 4HI) (formula: C<sub>27</sub>H<sub>32</sub>FN<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	B	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	C	1	Total	C	F	N	O	0	0
			36	27	1	3	5		
2	D	1	Total	C	F	N	O	0	0
			36	27	1	3	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		

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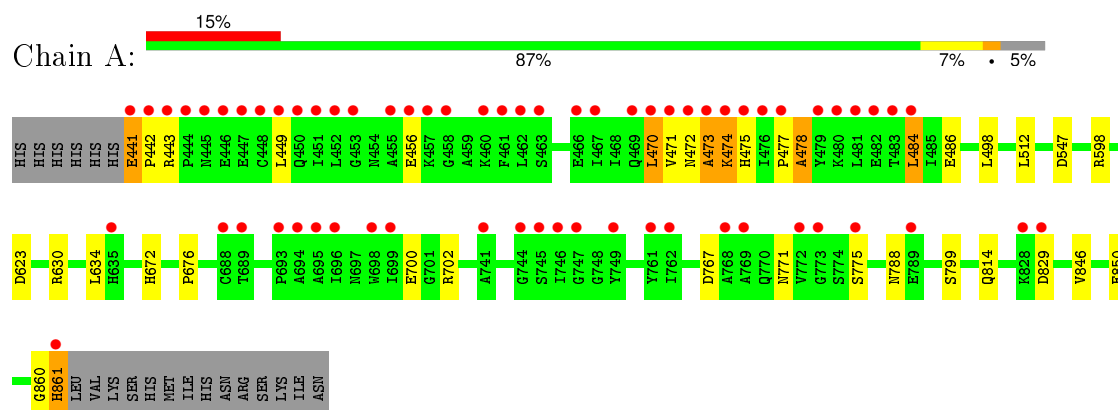
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	113	Total 113	O 113	0	0
3	C	89	Total 89	O 89	0	0
3	D	109	Total 109	O 109	0	0

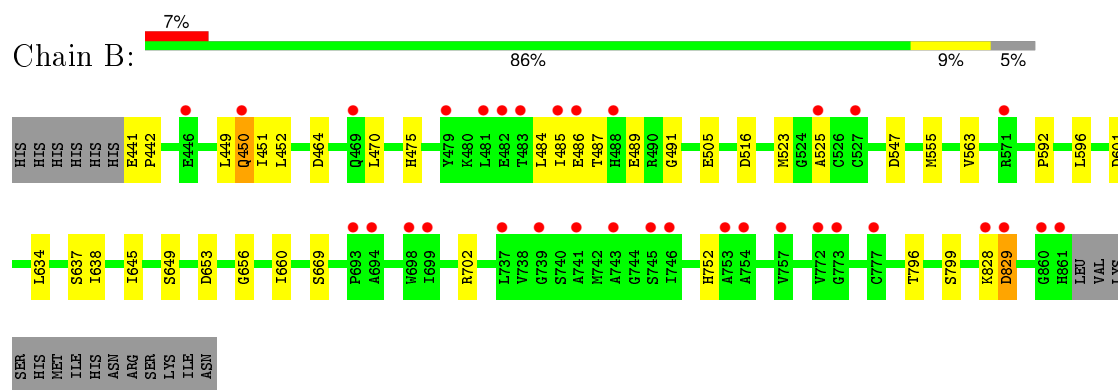
### 3 Residue-property plots [i](#)

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.

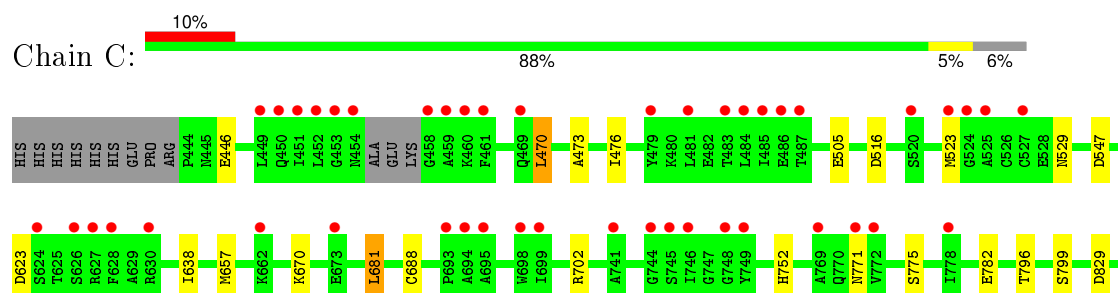
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

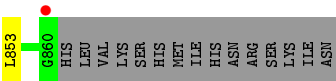


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

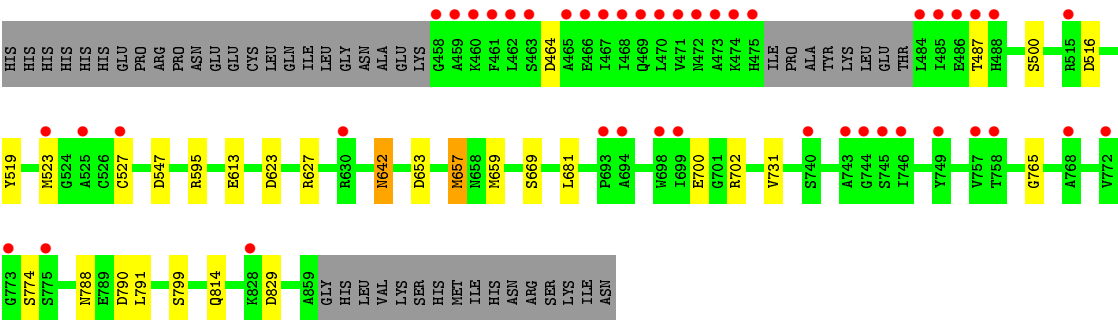
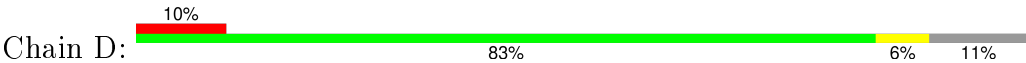


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase





● 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, $\alpha$ , $\beta$ , $\gamma$	73.93Å 174.38Å 76.08Å 90.00° 118.83° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.4 (50.00-2.10) 88.4 (38.16-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.217 , 0.252 0.220 , 0.253	Depositor DCC
$R_{free}$ test set	2646 reflections (3.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.3	EDS
Estimated twinning fraction	0.006 for -h-l,k,h 0.006 for l,k,-h-l 0.027 for h,-k,-h-l 0.027 for -h-l,-k,l 0.029 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 87274 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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:  
4HI

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	0.37	0/3179	0.63	4/4298 (0.1%)
1	B	0.37	0/3179	0.63	5/4298 (0.1%)
1	C	0.34	0/3116	0.60	4/4211 (0.1%)
1	D	0.36	0/2960	0.64	7/3999 (0.2%)
All	All	0.36	0/12434	0.62	20/16806 (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	A	623	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	547	ASP	CB-CG-OD2	5.84	123.56	118.30
1	D	547	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	653	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	653	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	464	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	623	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	829	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	767	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	516	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	790	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	829	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	464	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	623	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	516	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	547	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	829	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	547	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	829	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	516	ASP	CB-CG-OD2	5.00	122.80	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	15	0
1	B	3133	0	3167	14	0
1	C	3073	0	3110	8	0
1	D	2920	0	2957	10	0
2	B	72	0	62	3	0
2	C	36	0	31	0	0
2	D	36	0	31	0	0
3	A	109	0	0	0	0
3	B	113	0	0	0	0
3	C	89	0	0	1	0
3	D	109	0	0	2	0
All	All	12823	0	12525	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:A:470:LEU:O	1:A:474:LYS:O	2.07	0.72
1:C:771:ASN:OD1	1:C:775:SER:OG	2.11	0.67
1:B:555:MET:HE1	1:B:563:VAL:HA	1.81	0.60
1:A:471:VAL:HG11	1:A:498:LEU:HD21	1.83	0.60
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.86	0.57
1:D:595:ARG:HD2	1:D:681:LEU:HD22	1.86	0.57
1:A:860:GLY:O	1:A:861:HIS:HB2	2.05	0.57
1:D:642:ASN:N	1:D:642:ASN:HD22	2.01	0.57
2:B:2:4HI:H13B	2:B:2:4HI:H7	1.87	0.55
1:A:477:PRO:O	1:A:478:ALA:HB2	2.08	0.54
1:B:555:MET:CE	1:B:563:VAL:HA	2.38	0.54
1:D:657:MET:HG3	3:D:197:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ASN:OD1	1:A:775:SER:OG	2.27	0.53
2:B:2:4HI:H8A	2:B:2:4HI:H14B	1.92	0.52
1:A:472:ASN:O	1:A:473:ALA:CB	2.57	0.52
1:A:474:LYS:O	1:A:475:HIS:HB2	2.09	0.52
1:A:441:GLU:N	1:A:442:PRO:CD	2.72	0.52
1:B:449:LEU:HD11	1:B:475:HIS:ND1	2.26	0.50
1:A:477:PRO:O	1:A:478:ALA:CB	2.59	0.49
1:A:700:GLU:OE2	1:D:700:GLU:OE2	2.29	0.49
1:B:485:ILE:HD12	1:B:491:GLY:HA2	1.95	0.48
1:B:450:GLN:HG3	1:B:451:ILE:N	2.29	0.48
1:A:702:ARG:O	1:A:799:SER:HA	2.14	0.48
1:C:529:ASN:ND2	3:C:252:HOH:O	2.48	0.46
1:C:470:LEU:O	1:C:473:ALA:O	2.34	0.46
1:B:796:THR:HG21	1:C:638:ILE:O	2.16	0.46
1:B:555:MET:CE	1:B:563:VAL:HG22	2.46	0.46
1:B:638:ILE:O	1:C:796:THR:HG21	2.16	0.45
1:C:702:ARG:O	1:C:799:SER:HA	2.17	0.45
2:B:1:4HI:H13B	2:B:1:4HI:H7	1.98	0.45
1:D:519:TYR:O	1:D:523:MET:HG2	2.17	0.45
1:B:592:PRO:HD2	1:B:645:ILE:O	2.17	0.45
1:A:846:VAL:O	1:A:850:GLU:HG2	2.17	0.45
1:A:471:VAL:HG11	1:A:498:LEU:CD2	2.45	0.44
1:A:672:HIS:CD2	1:A:676:PRO:HA	2.52	0.44
1:D:700:GLU:OE1	3:D:369:HOH:O	2.21	0.44
1:D:774:SER:HA	1:D:799:SER:O	2.19	0.43
1:B:702:ARG:O	1:B:799:SER:HA	2.19	0.43
1:A:449:LEU:HD11	1:A:475:HIS:ND1	2.34	0.43
1:C:752:HIS:CD2	1:C:853:LEU:HD23	2.53	0.43
1:B:656:GLY:O	1:B:660:ILE:HG12	2.19	0.42
1:D:702:ARG:O	1:D:799:SER:HA	2.20	0.42
1:D:765:GLY:HA2	1:D:814:GLN:HG2	2.03	0.41
1:B:596:LEU:HB3	1:B:601:ASP:HB2	2.02	0.41
1:B:555:MET:HE2	1:B:563:VAL:HG22	2.03	0.40
1:B:441:GLU:N	1:B:442:PRO:CD	2.85	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%)	18 (4%)	3 (1%)	26	21
1	B	419/441 (95%)	406 (97%)	12 (3%)	1 (0%)	52	53
1	C	410/441 (93%)	397 (97%)	13 (3%)	0	100	100
1	D	390/441 (88%)	377 (97%)	13 (3%)	0	100	100
All	All	1638/1764 (93%)	1578 (96%)	56 (3%)	4 (0%)	52	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ALA
1	A	478	ALA
1	A	484	LEU
1	B	525	ALA

### 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%)	321 (96%)	14 (4%)	36	35
1	B	335/355 (94%)	319 (95%)	16 (5%)	31	29
1	C	329/355 (93%)	319 (97%)	10 (3%)	48	51
1	D	312/355 (88%)	301 (96%)	11 (4%)	43	44
All	All	1311/1420 (92%)	1260 (96%)	51 (4%)	39	39

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	456	GLU
1	A	470	LEU
1	A	474	LYS
1	A	484	LEU
1	A	486	GLU
1	A	512	LEU
1	A	598	ARG
1	A	630	ARG
1	A	634	LEU
1	A	788	ASN
1	A	814	GLN
1	A	861	HIS
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	484	LEU
1	B	486	GLU
1	B	487	THR
1	B	489	GLU
1	B	505	GLU
1	B	523	MET
1	B	634	LEU
1	B	637	SER
1	B	649	SER
1	B	669	SER
1	B	752	HIS
1	B	828	LYS
1	B	829	ASP
1	C	446	GLU
1	C	470	LEU
1	C	476	ILE
1	C	505	GLU
1	C	523	MET
1	C	657	MET
1	C	670	LYS
1	C	681	LEU
1	C	688	CYS
1	C	782	GLU
1	D	487	THR
1	D	500	SER

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Mol	Chain	Res	Type
1	D	527	CYS
1	D	613	GLU
1	D	627	ARG
1	D	642	ASN
1	D	657	MET
1	D	659	MET
1	D	669	SER
1	D	788	ASN
1	D	791	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN
1	A	635	HIS
1	A	672	HIS
1	B	472	ASN
1	B	510	GLN
1	B	529	ASN
1	B	632	GLN
1	C	469	GLN
1	C	472	ASN
1	C	672	HIS
1	C	679	GLN
1	C	824	GLN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	788	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	4HI	B	1	-	31,38,38	0.60	0	38,52,52	1.64	4 (10%)
2	4HI	B	2	-	31,38,38	0.56	0	38,52,52	1.45	4 (10%)
2	4HI	C	4	-	31,38,38	0.54	0	38,52,52	1.50	2 (5%)
2	4HI	D	3	-	31,38,38	0.53	0	38,52,52	1.79	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	4HI	B	1	-	-	0/25/30/30	0/3/3/3
2	4HI	B	2	-	-	0/25/30/30	0/3/3/3
2	4HI	C	4	-	-	0/25/30/30	0/3/3/3
2	4HI	D	3	-	-	0/25/30/30	0/3/3/3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	3	4HI	C8-C7-N1	-8.30	105.29	112.29
2	B	1	4HI	C8-C7-N1	-7.02	106.37	112.29
2	B	2	4HI	C8-C7-N1	-5.54	107.62	112.29
2	C	4	4HI	C8-C7-N1	-5.47	107.67	112.29
2	C	4	4HI	C2-C12-C6	-3.23	123.89	130.43
2	B	2	4HI	C2-C12-C6	-3.15	124.05	130.43
2	D	3	4HI	C2-C12-C6	-3.14	124.06	130.43
2	B	1	4HI	C2-C12-C6	-2.65	125.06	130.43
2	B	2	4HI	N3-C5-N1	-2.22	109.58	115.21
2	D	3	4HI	N3-C5-N1	-2.14	109.80	115.21
2	B	1	4HI	N3-C5-N1	-2.09	109.91	115.21
2	B	1	4HI	C24-C30-C15	-2.02	119.97	122.87
2	B	2	4HI	C4-N2-C3	2.16	127.49	121.84
2	D	3	4HI	C4-N2-C3	2.33	127.94	121.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	4HI	1	0
2	B	2	4HI	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%)	0.63	64 (15%) <b>3</b> <b>4</b>	29, 42, 62, 69	0
1	B	421/441 (95%)	0.39	33 (7%) <b>16</b> <b>22</b>	29, 43, 56, 72	0
1	C	414/441 (93%)	0.64	46 (11%) <b>7</b> <b>10</b>	30, 46, 83, 103	0
1	D	394/441 (89%)	0.48	44 (11%) <b>7</b> <b>9</b>	29, 43, 82, 108	0
All	All	1650/1764 (93%)	0.54	187 (11%) <b>7</b> <b>9</b>	29, 43, 66, 108	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	GLY	12.0
1	D	461	PHE	8.3
1	D	470	LEU	8.1
1	C	452	LEU	7.8
1	B	861	HIS	7.1
1	C	525	ALA	7.0
1	D	459	ALA	7.0
1	D	475	HIS	6.9
1	C	453	GLY	6.7
1	C	524	GLY	6.7
1	A	479	TYR	6.5
1	A	452	LEU	6.4
1	C	481	LEU	6.3
1	D	485	ILE	6.3
1	D	527	CYS	6.1
1	C	484	LEU	5.8
1	D	484	LEU	5.8
1	D	486	GLU	5.7
1	C	483	THR	5.7
1	A	461	PHE	5.4
1	D	471	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	861	HIS	5.4
1	A	446	GLU	5.3
1	D	474	LYS	5.1
1	A	448	CYS	5.0
1	A	462	LEU	4.9
1	A	476	ILE	4.9
1	D	460	LYS	4.9
1	A	467	ILE	4.8
1	A	455	ALA	4.7
1	A	475	HIS	4.7
1	C	523	MET	4.7
1	C	527	CYS	4.6
1	A	445	ASN	4.5
1	C	461	PHE	4.5
1	C	451	ILE	4.5
1	D	469	GLN	4.4
1	B	828	LYS	4.2
1	A	473	ALA	4.2
1	A	470	LEU	4.2
1	A	450	GLN	4.1
1	C	450	GLN	4.0
1	A	447	GLU	4.0
1	C	746	ILE	4.0
1	C	487	THR	3.9
1	D	523	MET	3.9
1	C	748	GLY	3.8
1	B	772	VAL	3.8
1	C	485	ILE	3.8
1	A	444	PRO	3.7
1	A	746	ILE	3.7
1	C	449	LEU	3.7
1	A	449	LEU	3.7
1	D	462	LEU	3.7
1	B	829	ASP	3.7
1	C	454	ASN	3.6
1	A	477	PRO	3.6
1	A	474	LYS	3.6
1	A	471	VAL	3.5
1	A	481	LEU	3.5
1	A	828	LYS	3.5
1	A	772	VAL	3.5
1	A	463	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	699	ILE	3.4
1	D	746	ILE	3.4
1	D	525	ALA	3.4
1	A	451	ILE	3.4
1	C	486	GLU	3.4
1	B	488	HIS	3.4
1	B	446	GLU	3.3
1	C	628	PHE	3.3
1	C	772	VAL	3.3
1	C	458	GLY	3.3
1	A	457	LYS	3.3
1	A	689	THR	3.3
1	A	773	GLY	3.3
1	D	463	SER	3.3
1	A	741	ALA	3.2
1	D	772	VAL	3.2
1	B	527	CYS	3.2
1	A	458	GLY	3.2
1	D	744	GLY	3.1
1	A	483	THR	3.1
1	A	443	ARG	3.1
1	A	469	GLN	3.1
1	A	442	PRO	3.1
1	A	456	GLU	3.0
1	B	698	TRP	3.0
1	A	480	LYS	2.9
1	C	479	TYR	2.9
1	A	696	ILE	2.9
1	C	778	ILE	2.9
1	B	746	ILE	2.9
1	A	484	LEU	2.9
1	A	775	SER	2.8
1	C	627	ARG	2.8
1	A	693	PRO	2.8
1	D	693	PRO	2.8
1	A	460	LYS	2.8
1	A	769	ALA	2.8
1	D	768	ALA	2.8
1	B	482	GLU	2.7
1	D	745	SER	2.7
1	A	699	ILE	2.7
1	B	757	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	694	ALA	2.7
1	D	828	LYS	2.7
1	B	481	LEU	2.6
1	B	741	ALA	2.6
1	B	743	ALA	2.6
1	C	520	SER	2.6
1	A	698	TRP	2.6
1	B	479	TYR	2.6
1	C	662	LYS	2.6
1	C	469	GLN	2.6
1	C	626	SER	2.6
1	D	465	ALA	2.6
1	D	472	ASN	2.6
1	A	441	GLU	2.6
1	C	624	SER	2.5
1	A	695	ALA	2.5
1	D	694	ALA	2.5
1	D	467	ILE	2.5
1	C	771	ASN	2.5
1	D	515	ARG	2.5
1	C	699	ILE	2.5
1	A	761	TYR	2.5
1	B	693	PRO	2.5
1	B	777	CYS	2.5
1	C	741	ALA	2.4
1	A	635	HIS	2.4
1	A	789	GLU	2.4
1	A	453	GLY	2.4
1	B	739	GLY	2.4
1	B	860	GLY	2.4
1	A	482	GLU	2.4
1	D	757	VAL	2.4
1	D	698	TRP	2.4
1	B	754	ALA	2.4
1	B	483	THR	2.4
1	A	829	ASP	2.3
1	A	768	ALA	2.3
1	D	468	ILE	2.3
1	D	488	HIS	2.3
1	A	749	TYR	2.3
1	A	762	ILE	2.3
1	A	466	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	450	GLN	2.3
1	B	694	ALA	2.3
1	B	773	GLY	2.2
1	D	699	ILE	2.2
1	B	753	ALA	2.2
1	C	769	ALA	2.2
1	D	743	ALA	2.2
1	B	745	SER	2.2
1	C	459	ALA	2.2
1	C	749	TYR	2.2
1	C	744	GLY	2.2
1	D	630	ARG	2.2
1	B	737	LEU	2.2
1	C	695	ALA	2.2
1	D	487	THR	2.1
1	D	473	ALA	2.1
1	B	469	GLN	2.1
1	D	466	GLU	2.1
1	A	472	ASN	2.1
1	C	698	TRP	2.1
1	C	673	GLU	2.1
1	C	745	SER	2.1
1	C	860	GLY	2.1
1	D	740	SER	2.1
1	B	525	ALA	2.1
1	D	749	TYR	2.1
1	C	630	ARG	2.1
1	D	758	THR	2.1
1	A	744	GLY	2.1
1	A	745	SER	2.1
1	B	486	GLU	2.1
1	D	773	GLY	2.0
1	D	775	SER	2.0
1	C	694	ALA	2.0
1	B	571	ARG	2.0
1	C	693	PRO	2.0
1	A	688	CYS	2.0
1	A	747	GLY	2.0
1	B	485	ILE	2.0
1	C	460	LYS	2.0

## 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	4HI	D	3	36/36	0.89	0.14	0.62	31,41,44,47	0
2	4HI	C	4	36/36	0.87	0.15	0.23	33,45,47,51	0
2	4HI	B	2	36/36	0.94	0.13	-0.53	29,37,43,46	0
2	4HI	B	1	36/36	0.94	0.11	-0.60	32,41,42,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.