



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:00 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 validation 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>

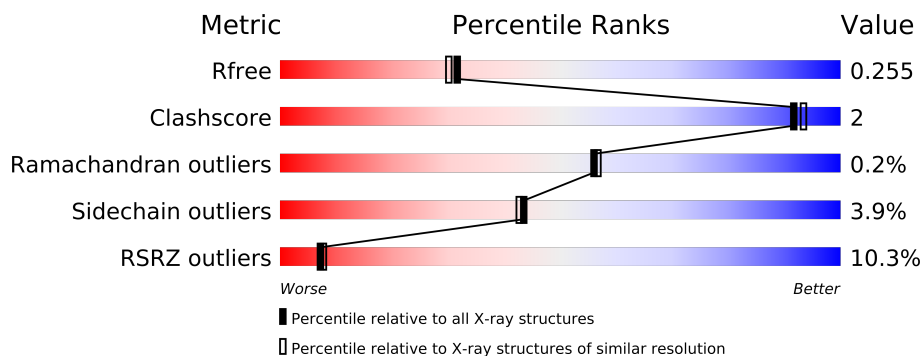
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
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 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 ≥ 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 12823 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	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:

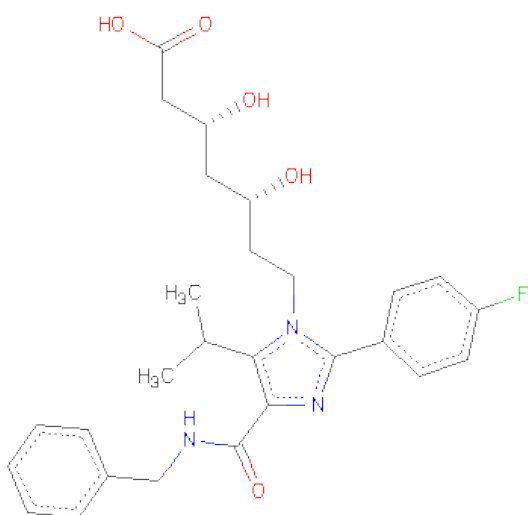
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered	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-DIHYDROXYHEPTANOICACID (three-letter code: 4HI) (formula: C₂₇H₃₂FN₃O₅).



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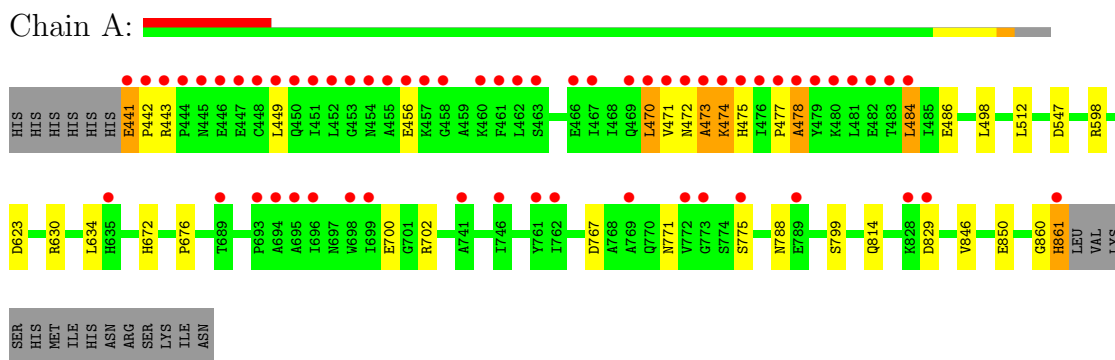
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	113	Total 113	O 113	0	0
3	C	89	Total 89	O 89	0	0
3	D	109	Total 109	O 109	0	0

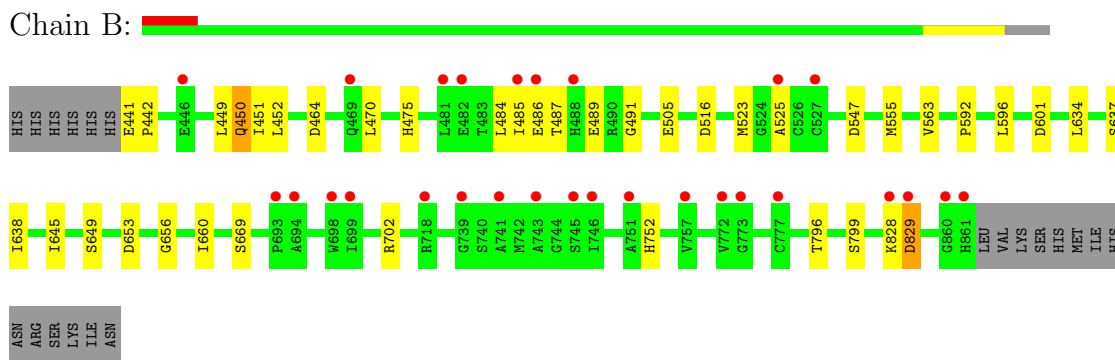
3 Residue-property plots

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.

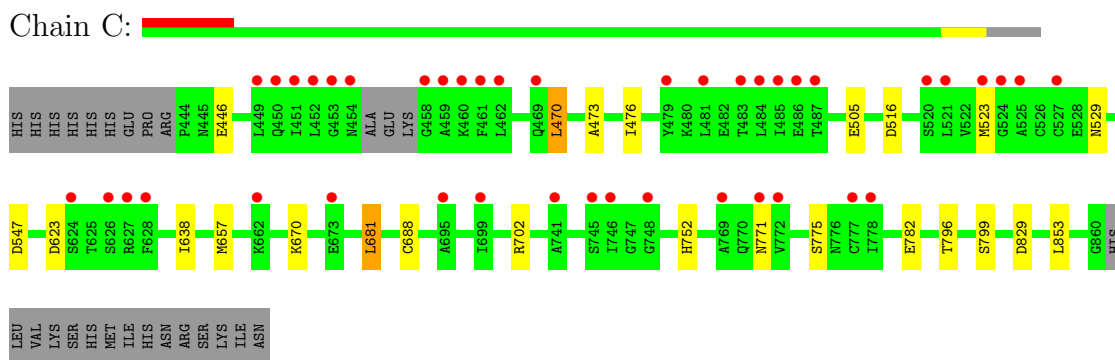
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase



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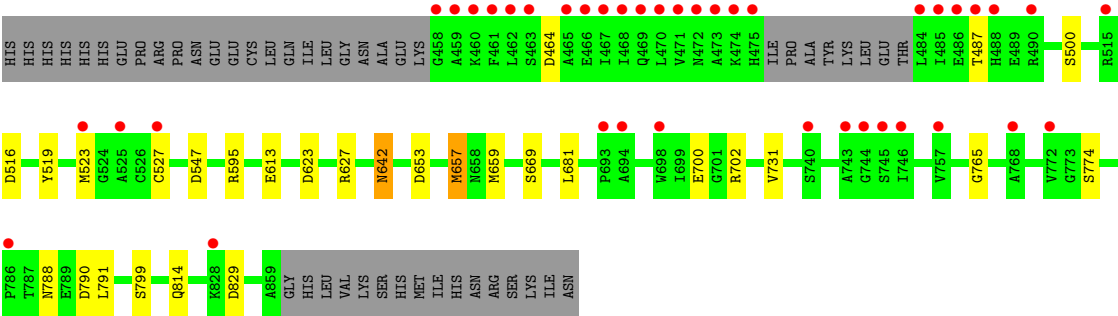


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.252 0.220 , 0.255	Depositor DCC
R_{free} test set	2647 reflections (3.13%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.6	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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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 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	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

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

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	30	23
1	B	419/441 (95%)	406 (97%)	12 (3%)	1 (0%)	56	57
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%)	56	57

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%)	40	38
1	B	335/355 (94%)	319 (95%)	16 (5%)	35	32
1	C	329/355 (93%)	319 (97%)	10 (3%)	53	55
1	D	312/355 (88%)	301 (96%)	11 (4%)	48	48
All	All	1311/1420 (92%)	1260 (96%)	51 (4%)	43	43

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
1	D	527	CYS

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Mol	Chain	Res	Type
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 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	4HI	B	1	-	38,38,38	0.69	0	52,52,52	1.77	9 (17%)
2	4HI	B	2	-	38,38,38	0.65	0	52,52,52	1.74	10 (19%)
2	4HI	C	4	-	38,38,38	0.66	1 (2%)	52,52,52	1.76	9 (17%)
2	4HI	D	3	-	38,38,38	0.65	0	52,52,52	1.88	8 (15%)

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	-	-	0/28/30/30	0/3/3/3
2	4HI	B	2	-	-	0/28/30/30	0/3/3/3
2	4HI	C	4	-	-	0/28/30/30	0/3/3/3
2	4HI	D	3	-	-	0/28/30/30	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	4HI	C2-N3	-2.03	1.33	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	4HI	C8-C7-N1	-8.64	105.29	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	4HI	C8-C7-N1	-7.30	106.37	112.31
2	B	2	4HI	C8-C7-N1	-5.77	107.62	112.31
2	C	4	4HI	C8-C7-N1	-5.70	107.67	112.31
2	B	2	4HI	C12-C2-C3	-4.26	122.62	130.70
2	B	2	4HI	C27-C5-N1	3.84	130.12	124.76
2	B	1	4HI	C7-C8-C9	3.80	117.43	113.82
2	C	4	4HI	C12-C2-C3	-3.78	123.53	130.70
2	D	3	4HI	C12-C2-C3	-3.65	123.77	130.70
2	C	4	4HI	C7-C8-C9	3.65	117.28	113.82
2	D	3	4HI	C27-C5-N1	3.61	129.81	124.76
2	B	1	4HI	C12-C2-C3	-3.46	124.14	130.70
2	C	4	4HI	C2-C12-C6	-3.30	123.89	130.68
2	C	4	4HI	C27-C5-N1	3.25	129.30	124.76
2	B	2	4HI	C2-C12-C6	-3.23	124.05	130.68
2	D	3	4HI	C2-C12-C6	-3.22	124.06	130.68
2	B	2	4HI	C3-C2-N3	3.13	128.16	121.14
2	D	3	4HI	C7-C8-C9	3.09	116.75	113.82
2	B	2	4HI	C7-C8-C9	3.05	116.72	113.82
2	D	3	4HI	C6-C12-N1	3.02	130.31	122.43
2	B	1	4HI	C27-C5-N1	2.93	128.84	124.76
2	C	4	4HI	C6-C12-N1	2.84	129.84	122.43
2	C	4	4HI	C3-C2-N3	2.77	127.34	121.14
2	B	2	4HI	C6-C12-N1	2.77	129.65	122.43
2	C	4	4HI	C12-N1-C5	-2.75	107.36	109.76
2	B	1	4HI	C2-C12-C6	-2.73	125.06	130.68
2	B	1	4HI	C6-C12-N1	2.48	128.91	122.43
2	D	3	4HI	C3-C2-N3	2.47	126.68	121.14
2	B	1	4HI	C3-C2-N3	2.40	126.51	121.14
2	B	1	4HI	C12-N1-C5	-2.38	107.68	109.76
2	D	3	4HI	C4-N2-C3	2.26	127.94	121.69
2	B	2	4HI	C12-N1-C5	-2.26	107.78	109.76
2	B	2	4HI	C2-C3-N2	2.17	117.49	115.83
2	C	4	4HI	C2-C3-N2	2.16	117.49	115.83
2	B	1	4HI	C24-C30-C15	-2.16	119.97	122.90
2	B	2	4HI	C4-N2-C3	2.10	127.49	121.69

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%)	0.59	60 (14%) 3 4	29, 42, 62, 69	0
1	B	421/441 (95%)	0.36	28 (6%) 17 19	29, 43, 56, 72	0
1	C	414/441 (93%)	0.62	42 (10%) 7 8	30, 46, 83, 103	0
1	D	394/441 (89%)	0.49	40 (10%) 7 8	29, 43, 82, 108	0
All	All	1650/1764 (93%)	0.51	170 (10%) 7 8	29, 43, 66, 108	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	GLY	11.1
1	D	470	LEU	8.4
1	C	452	LEU	8.4
1	C	525	ALA	8.0
1	D	475	HIS	7.6
1	D	461	PHE	7.5
1	D	459	ALA	7.0
1	D	485	ILE	7.0
1	A	452	LEU	6.4
1	D	484	LEU	6.3
1	B	861	HIS	6.1
1	C	524	GLY	6.1
1	D	486	GLU	6.0
1	D	474	LYS	5.9
1	D	471	VAL	5.7
1	A	479	TYR	5.7
1	C	453	GLY	5.6
1	C	484	LEU	5.4
1	C	483	THR	5.4
1	D	527	CYS	5.3
1	A	861	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	481	LEU	5.1
1	C	451	ILE	4.7
1	A	476	ILE	4.7
1	D	460	LYS	4.7
1	A	446	GLU	4.5
1	A	475	HIS	4.5
1	A	455	ALA	4.5
1	C	450	GLN	4.4
1	A	461	PHE	4.4
1	A	462	LEU	4.4
1	C	449	LEU	4.2
1	A	448	CYS	4.2
1	C	461	PHE	4.2
1	A	449	LEU	4.1
1	C	485	ILE	4.1
1	A	473	ALA	4.1
1	C	487	THR	4.0
1	C	523	MET	4.0
1	A	450	GLN	4.0
1	B	828	LYS	3.9
1	A	445	ASN	3.8
1	D	469	GLN	3.8
1	A	458	GLY	3.6
1	C	527	CYS	3.6
1	C	486	GLU	3.6
1	A	467	ILE	3.6
1	C	748	GLY	3.6
1	A	447	GLU	3.5
1	A	470	LEU	3.5
1	C	746	ILE	3.5
1	B	488	HIS	3.5
1	B	527	CYS	3.5
1	B	829	ASP	3.5
1	D	525	ALA	3.5
1	A	474	LYS	3.3
1	D	523	MET	3.3
1	A	444	PRO	3.3
1	A	828	LYS	3.2
1	D	772	VAL	3.2
1	D	462	LEU	3.2
1	B	772	VAL	3.2
1	B	699	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	772	VAL	3.2
1	A	477	PRO	3.2
1	A	746	ILE	3.2
1	D	746	ILE	3.1
1	A	483	THR	3.1
1	A	741	ALA	3.1
1	B	446	GLU	3.1
1	C	458	GLY	3.1
1	A	451	ILE	3.1
1	C	628	PHE	3.0
1	A	471	VAL	3.0
1	A	773	GLY	3.0
1	A	453	GLY	3.0
1	D	487	THR	3.0
1	A	469	GLN	3.0
1	D	465	ALA	2.9
1	A	442	PRO	2.9
1	A	457	LYS	2.9
1	A	463	SER	2.9
1	A	480	LYS	2.9
1	D	473	ALA	2.9
1	B	698	TRP	2.9
1	A	689	THR	2.9
1	D	463	SER	2.9
1	C	772	VAL	2.8
1	D	744	GLY	2.8
1	C	627	ARG	2.8
1	A	775	SER	2.7
1	A	481	LEU	2.7
1	C	479	TYR	2.7
1	A	456	GLU	2.7
1	C	778	ILE	2.6
1	A	761	TYR	2.6
1	D	745	SER	2.6
1	D	515	ARG	2.6
1	C	662	LYS	2.6
1	D	828	LYS	2.6
1	D	768	ALA	2.5
1	D	693	PRO	2.5
1	C	454	ASN	2.5
1	C	520	SER	2.5
1	C	626	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	460	LYS	2.4
1	B	482	GLU	2.4
1	D	466	GLU	2.4
1	A	696	ILE	2.4
1	C	771	ASN	2.4
1	B	757	VAL	2.4
1	A	441	GLU	2.4
1	C	624	SER	2.4
1	A	482	GLU	2.4
1	C	469	GLN	2.4
1	A	484	LEU	2.3
1	A	443	ARG	2.3
1	D	757	VAL	2.3
1	C	521	LEU	2.3
1	A	635	HIS	2.3
1	B	693	PRO	2.3
1	D	468	ILE	2.3
1	B	469	GLN	2.3
1	B	481	LEU	2.3
1	D	694	ALA	2.2
1	A	829	ASP	2.2
1	A	478	ALA	2.2
1	B	741	ALA	2.2
1	B	773	GLY	2.2
1	C	699	ILE	2.2
1	A	698	TRP	2.2
1	D	786	PRO	2.2
1	D	743	ALA	2.2
1	B	486	GLU	2.2
1	D	467	ILE	2.2
1	B	860	GLY	2.2
1	A	694	ALA	2.2
1	B	525	ALA	2.2
1	A	472	ASN	2.2
1	A	699	ILE	2.2
1	A	769	ALA	2.2
1	A	454	ASN	2.2
1	C	745	SER	2.2
1	A	762	ILE	2.2
1	A	693	PRO	2.2
1	D	740	SER	2.2
1	D	490	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	789	GLU	2.1
1	B	746	ILE	2.1
1	B	743	ALA	2.1
1	D	488	HIS	2.1
1	D	698	TRP	2.1
1	B	739	GLY	2.1
1	B	694	ALA	2.1
1	C	459	ALA	2.1
1	C	673	GLU	2.1
1	C	741	ALA	2.1
1	C	769	ALA	2.1
1	B	485	ILE	2.0
1	B	718	ARG	2.0
1	A	695	ALA	2.0
1	D	472	ASN	2.0
1	C	460	LYS	2.0
1	C	777	CYS	2.0
1	A	466	GLU	2.0
1	B	745	SER	2.0
1	B	751	ALA	2.0
1	C	695	ALA	2.0
1	C	462	LEU	2.0
1	B	777	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, 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	4HI	D	3	36/36	0.14	0.52	31,41,44,47	0
2	4HI	C	4	36/36	0.15	0.39	33,45,47,51	0
2	4HI	B	2	36/36	0.13	-0.39	29,37,43,46	0
2	4HI	B	1	36/36	0.10	-0.76	32,41,42,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.