



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 AM GMT

PDB ID : 3CCT
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 : 2.12 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
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

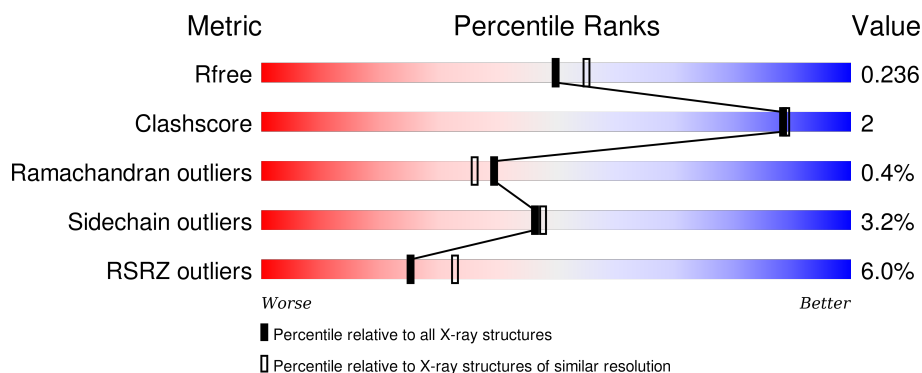
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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. 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>6%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>
1	B	441	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	C	441	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
1	D	441	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12845 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	417	Total	C	N	O	S	0	0	0
			3096	1929	542	595	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

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- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	96	Total O 96 96	0	0

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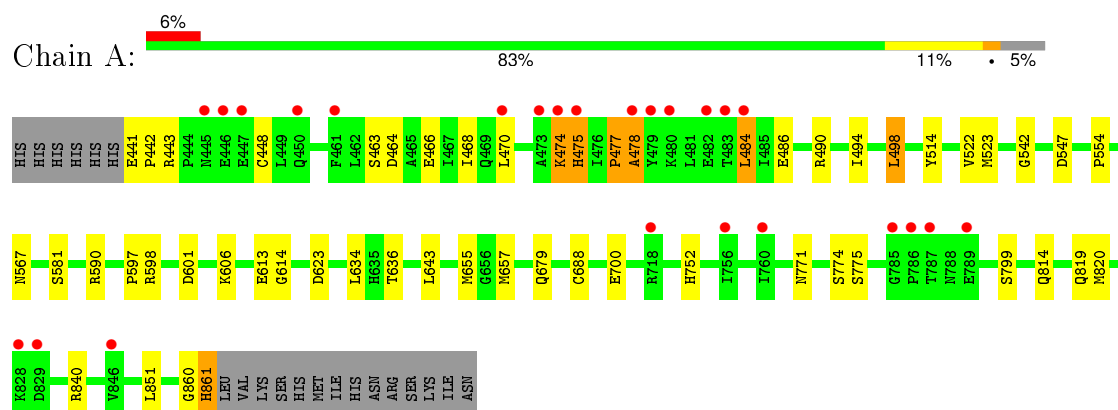
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	113	Total 113	O 113	0	0
3	C	83	Total 83	O 83	0	0
3	D	103	Total 103	O 103	0	0

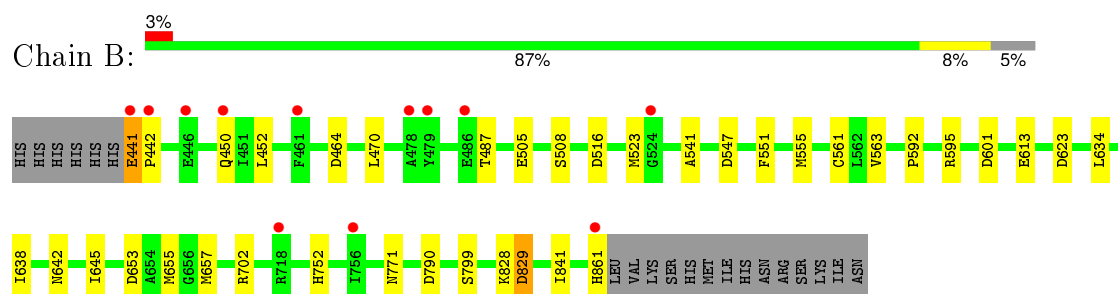
3 Residue-property plots [i](#)

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.

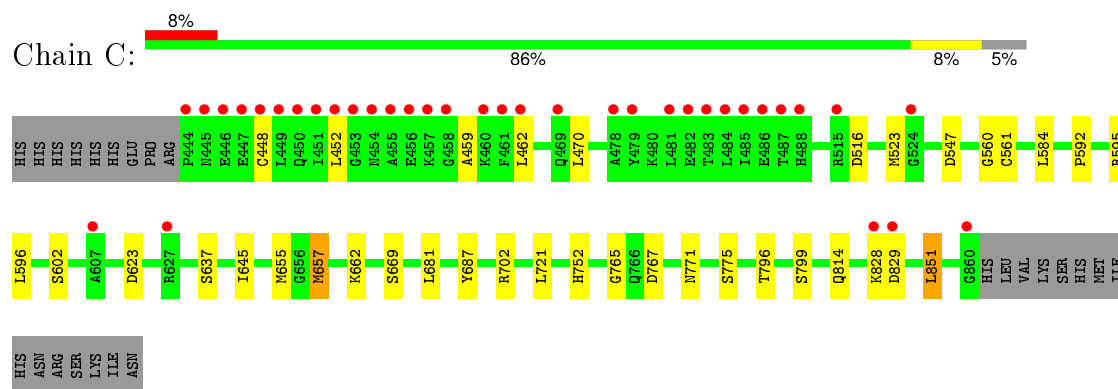
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



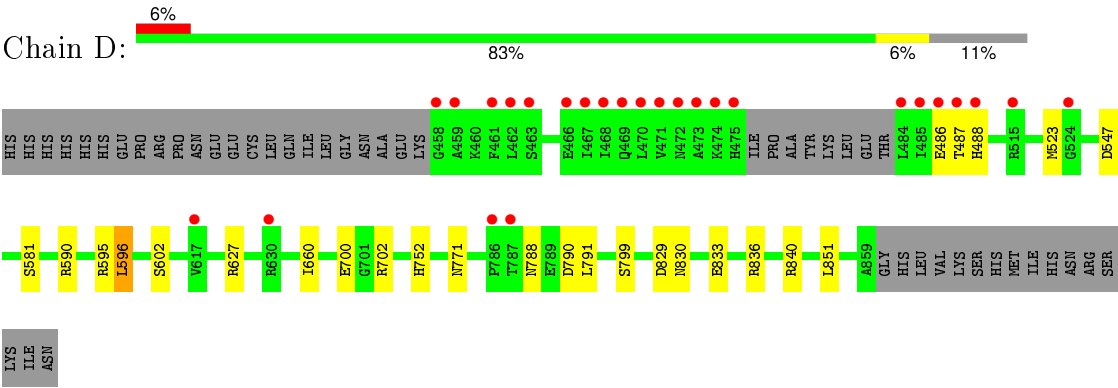
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- 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, α , β , γ	73.94Å 173.51Å 76.40Å 90.00° 119.18° 90.00°	Depositor
Resolution (Å)	30.00 – 2.12 28.92 – 2.12	Depositor EDS
% Data completeness (in resolution range)	88.7 (30.00-2.12) 88.7 (28.92-2.12)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.236 0.200 , 0.236	Depositor DCC
R_{free} test set	8707 reflections (11.49%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.025 for h,-k,-h-l 0.025 for l,-k,h 0.023 for -h-l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 86825 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12845	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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:
3HI

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	0.45	0/3179	0.68	4/4298 (0.1%)
1	B	0.45	0/3179	0.66	8/4298 (0.2%)
1	C	0.43	0/3140	0.64	5/4244 (0.1%)
1	D	0.44	0/2960	0.67	4/3999 (0.1%)
All	All	0.44	0/12458	0.66	21/16839 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	547	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	464	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	547	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	547	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	547	ASP	CB-CG-OD2	5.65	123.38	118.30
1	C	623	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	829	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	464	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	516	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	790	ASP	CB-CG-OD2	5.36	123.13	118.30
1	C	767	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	516	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	836	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	D	829	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	623	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	601	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	601	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	829	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	790	ASP	CB-CG-OD2	5.03	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	653	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	26	0
1	B	3133	0	3167	12	0
1	C	3096	0	3135	16	0
1	D	2920	0	2957	10	0
2	B	84	0	66	4	0
2	C	42	0	33	0	0
2	D	42	0	33	0	0
3	A	96	0	0	1	0
3	B	113	0	0	0	0
3	C	83	0	0	0	0
3	D	103	0	0	1	0
All	All	12845	0	12558	62	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 (62) 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:655:MET:SD	1:A:657:MET:HG2	2.19	0.83
1:C:771:ASN:OD1	1:C:775:SER:OG	2.03	0.74
1:B:555:MET:HE3	1:B:563:VAL:HG22	1.71	0.71
1:A:700:GLU:OE2	1:D:700:GLU:OE2	2.10	0.69
1:A:679:GLN:NE2	3:A:343:HOH:O	2.27	0.68
2:B:1:3HI:H7	2:B:1:3HI:H13B	1.81	0.61
1:A:860:GLY:O	1:A:861:HIS:HB2	2.00	0.61
1:D:596:LEU:HD13	1:D:602:SER:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:MET:SD	1:C:657:MET:HG2	2.43	0.58
1:A:636:THR:HG23	1:A:643:LEU:HD11	1.85	0.58
1:B:655:MET:SD	1:B:657:MET:HG2	2.46	0.55
1:D:627:ARG:HG3	3:D:111:HOH:O	2.06	0.55
1:A:522:VAL:HG12	1:A:523:MET:HE2	1.88	0.55
1:A:477:PRO:O	1:A:478:ALA:HB2	2.07	0.54
1:C:637:SER:HG	1:C:687:TYR:HH	1.56	0.54
1:A:468:ILE:HG12	1:A:498:LEU:CD1	2.38	0.54
1:B:441:GLU:N	1:B:442:PRO:CD	2.71	0.54
1:A:468:ILE:HG12	1:A:498:LEU:HD11	1.91	0.52
1:A:819:GLN:HB3	1:B:508:SER:HB3	1.91	0.52
1:A:771:ASN:OD1	1:A:775:SER:OG	2.28	0.52
1:C:596:LEU:HD13	1:C:602:SER:HA	1.91	0.51
1:A:774:SER:HA	1:A:799:SER:O	2.11	0.51
1:A:542:GLY:H	1:A:567:ASN:ND2	2.09	0.51
2:B:1:3HI:H8A	2:B:1:3HI:H14B	1.94	0.50
1:B:592:PRO:HD2	1:B:645:ILE:O	2.13	0.48
1:D:702:ARG:O	1:D:799:SER:HA	2.13	0.48
1:A:490:ARG:O	1:A:494:ILE:HG12	2.13	0.48
1:A:636:THR:CG2	1:A:643:LEU:HD11	2.42	0.47
1:C:702:ARG:O	1:C:799:SER:HA	2.15	0.47
1:A:474:LYS:O	1:A:475:HIS:CB	2.63	0.47
1:A:441:GLU:N	1:A:442:PRO:CD	2.78	0.47
1:B:702:ARG:O	1:B:799:SER:HA	2.14	0.46
1:A:606:LYS:HG3	1:A:636:THR:HG21	1.98	0.46
1:A:474:LYS:O	1:A:475:HIS:CG	2.69	0.45
1:D:581:SER:OG	1:D:840:ARG:HD2	2.17	0.44
1:A:477:PRO:O	1:A:478:ALA:CB	2.65	0.44
1:C:452:LEU:HD21	1:C:459:ALA:HB2	1.99	0.44
1:A:448:CYS:SG	1:A:466:GLU:HG2	2.58	0.44
1:A:554:PRO:HB3	1:A:820:MET:HE3	1.99	0.44
1:A:581:SER:OG	1:A:840:ARG:HD2	2.19	0.43
1:C:592:PRO:HD2	1:C:645:ILE:O	2.19	0.43
2:B:2:3HI:O1	2:B:2:3HI:H13B	2.17	0.43
1:B:541:ALA:HB2	1:B:555:MET:CE	2.49	0.43
1:B:561:CYS:HB3	2:B:2:3HI:O2	2.18	0.43
1:C:721:LEU:CD1	1:C:851:LEU:HD22	2.49	0.43
1:A:597:PRO:O	1:A:598:ARG:HD3	2.19	0.43
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.85	0.43
1:B:638:ILE:HD12	1:C:584:LEU:HD22	2.00	0.42
1:B:638:ILE:O	1:C:796:THR:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:GLY:CA	1:C:814:GLN:HG2	2.49	0.42
1:B:551:PHE:CE2	1:B:841:ILE:HD11	2.55	0.42
1:C:765:GLY:HA2	1:C:814:GLN:HG2	2.02	0.42
1:D:590:ARG:HB2	1:D:660:ILE:HG22	2.02	0.41
1:A:613:GLU:HG2	1:A:614:GLY:N	2.35	0.41
1:C:448:CYS:SG	1:C:462:LEU:HD22	2.60	0.41
1:B:595:ARG:HD2	1:B:642:ASN:OD1	2.20	0.41
1:D:488:HIS:HD2	1:D:523:MET:HG3	1.85	0.41
1:C:771:ASN:HB3	1:D:771:ASN:HD21	1.86	0.41
1:D:791:LEU:C	1:D:791:LEU:HD23	2.42	0.40
1:D:830:ASN:O	1:D:833:GLU:HB2	2.21	0.40
1:C:560:GLY:O	1:C:561:CYS:HB2	2.22	0.40
1:C:828:LYS:H	1:C:828:LYS:HG2	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	400 (96%)	13 (3%)	6 (1%)	14	7
1	B	419/441 (95%)	403 (96%)	16 (4%)	0	100	100
1	C	415/441 (94%)	395 (95%)	20 (5%)	0	100	100
1	D	390/441 (88%)	376 (96%)	14 (4%)	0	100	100
All	All	1643/1764 (93%)	1574 (96%)	63 (4%)	6 (0%)	39	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	LEU
1	A	475	HIS

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Mol	Chain	Res	Type
1	A	478	ALA
1	A	474	LYS
1	A	477	PRO
1	A	514	TYR

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%)	42	42
1	B	335/355 (94%)	321 (96%)	14 (4%)	36	35
1	C	331/355 (93%)	322 (97%)	9 (3%)	52	55
1	D	312/355 (88%)	305 (98%)	7 (2%)	60	63
All	All	1313/1420 (92%)	1271 (97%)	42 (3%)	46	48

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	A	463	SER
1	A	470	LEU
1	A	484	LEU
1	A	486	GLU
1	A	498	LEU
1	A	634	LEU
1	A	688	CYS
1	A	752	HIS
1	A	814	GLN
1	A	851	LEU
1	A	861	HIS
1	B	441	GLU
1	B	450	GLN
1	B	452	LEU
1	B	470	LEU
1	B	487	THR

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Mol	Chain	Res	Type
1	B	505	GLU
1	B	523	MET
1	B	613	GLU
1	B	634	LEU
1	B	752	HIS
1	B	771	ASN
1	B	828	LYS
1	B	829	ASP
1	B	861	HIS
1	C	470	LEU
1	C	523	MET
1	C	595	ARG
1	C	657	MET
1	C	662	LYS
1	C	669	SER
1	C	681	LEU
1	C	752	HIS
1	C	851	LEU
1	D	486	GLU
1	D	487	THR
1	D	595	ARG
1	D	596	LEU
1	D	752	HIS
1	D	788	ASN
1	D	851	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	488	HIS
1	A	510	GLN
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN
1	A	635	HIS
1	B	450	GLN
1	B	472	ASN
1	B	510	GLN
1	B	819	GLN
1	C	472	ASN
1	C	679	GLN

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Mol	Chain	Res	Type
1	D	488	HIS
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	788	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	3HI	B	1	-	40,45,45	0.98	2 (5%)	52,63,63	1.71	9 (17%)
2	3HI	B	2	-	40,45,45	1.02	2 (5%)	52,63,63	1.61	8 (15%)
2	3HI	C	4	-	40,45,45	1.02	2 (5%)	52,63,63	1.52	6 (11%)
2	3HI	D	3	-	40,45,45	1.18	1 (2%)	52,63,63	1.57	9 (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	3HI	B	1	-	-	0/27/33/33	0/4/4/4
2	3HI	B	2	-	-	0/27/33/33	0/4/4/4
2	3HI	C	4	-	-	0/27/33/33	0/4/4/4
2	3HI	D	3	-	-	0/27/33/33	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	3HI	C1-C2	-2.79	1.37	1.42
2	B	2	3HI	C1-C2	-2.30	1.38	1.42
2	C	4	3HI	C1-C2	-2.01	1.38	1.42
2	B	1	3HI	C1-C5	4.45	1.46	1.40
2	B	2	3HI	C1-C5	4.76	1.46	1.40
2	C	4	3HI	C1-C5	4.82	1.46	1.40
2	D	3	3HI	C1-C5	6.03	1.48	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	3HI	C8-C7-N1	-4.25	108.70	112.29
2	D	3	3HI	O1-C3-C2	-3.86	115.20	120.80
2	B	1	3HI	C2-C12-C6	-3.67	122.99	130.43
2	C	4	3HI	C21-C27-C5	-3.62	114.00	120.43
2	B	2	3HI	C21-C27-C5	-3.61	114.01	120.43
2	B	2	3HI	O1-C3-C2	-3.35	115.94	120.80
2	B	1	3HI	C8-C7-N1	-3.06	109.71	112.29
2	B	2	3HI	C10-C9-C8	-3.05	107.02	112.26
2	C	4	3HI	O1-C3-C2	-3.03	116.41	120.80
2	B	1	3HI	C10-C11-C35	-2.96	107.29	112.94
2	C	4	3HI	C10-C11-C35	-2.41	108.34	112.94
2	D	3	3HI	C10-C9-C8	-2.41	108.13	112.26
2	D	3	3HI	C21-C27-C5	-2.19	116.55	120.43
2	D	3	3HI	C9-C10-C11	-2.16	111.18	114.18
2	B	1	3HI	O1-C3-C2	-2.14	117.70	120.80
2	B	1	3HI	C7-N1-C5	-2.01	121.48	124.87
2	B	1	3HI	C7-N1-C12	2.48	129.26	124.74
2	B	2	3HI	C23-C26-C32	2.50	121.54	119.63
2	B	1	3HI	C2-C3-N2	2.59	119.94	114.88
2	D	3	3HI	O2-C26-C32	2.60	120.35	116.75
2	B	2	3HI	O2-C26-C32	2.77	120.59	116.75
2	C	4	3HI	C18-C27-C5	2.80	125.40	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	3HI	C2-C3-N2	2.89	120.52	114.88
2	B	1	3HI	O2-C26-C32	2.91	120.79	116.75
2	D	3	3HI	C23-C26-C32	3.10	122.00	119.63
2	B	2	3HI	C18-C27-C5	3.11	125.97	120.43
2	C	4	3HI	C2-C3-N2	3.35	121.42	114.88
2	D	3	3HI	C2-C3-N2	3.70	122.09	114.88
2	D	3	3HI	C27-C5-N1	3.77	128.96	123.22
2	C	4	3HI	C27-C5-N1	4.09	129.45	123.22
2	B	2	3HI	C27-C5-N1	4.77	130.49	123.22
2	B	1	3HI	C27-C5-N1	7.26	134.26	123.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	3HI	2	0
2	B	2	3HI	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, 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%)	0.20	25 (5%) 26 33	20, 33, 75, 98	0
1	B	421/441 (95%)	0.03	12 (2%) 55 63	20, 33, 51, 84	0
1	C	417/441 (94%)	0.44	36 (8%) 13 18	20, 37, 83, 95	0
1	D	394/441 (89%)	0.18	26 (6%) 22 29	19, 32, 73, 99	0
All	All	1653/1764 (93%)	0.21	99 (5%) 25 33	19, 33, 72, 99	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	484	LEU	7.8
1	D	475	HIS	7.8
1	C	455	ALA	7.7
1	D	461	PHE	7.3
1	B	479	TYR	6.7
1	C	461	PHE	6.3
1	C	453	GLY	6.2
1	C	483	THR	6.1
1	C	452	LEU	6.0
1	D	470	LEU	5.8
1	A	483	THR	5.6
1	D	485	ILE	5.6
1	C	484	LEU	5.3
1	D	458	GLY	5.3
1	A	479	TYR	5.1
1	C	456	GLU	5.0
1	D	486	GLU	5.0
1	D	474	LYS	4.9
1	C	479	TYR	4.7
1	C	457	LYS	4.6
1	A	786	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	446	GLU	4.4
1	A	482	GLU	4.1
1	C	451	ILE	4.0
1	C	444	PRO	4.0
1	C	460	LYS	3.9
1	C	524	GLY	3.9
1	D	524	GLY	3.9
1	C	449	LEU	3.9
1	C	462	LEU	3.9
1	C	458	GLY	3.9
1	D	471	VAL	3.8
1	D	459	ALA	3.8
1	B	478	ALA	3.7
1	A	450	GLN	3.6
1	D	469	GLN	3.5
1	A	473	ALA	3.4
1	A	828	LYS	3.4
1	B	861	HIS	3.3
1	A	480	LYS	3.3
1	D	473	ALA	3.3
1	C	487	THR	3.3
1	C	627	ARG	3.3
1	A	787	THR	3.2
1	A	474	LYS	3.2
1	D	787	THR	3.2
1	C	481	LEU	3.2
1	C	450	GLN	3.2
1	A	445	ASN	3.2
1	C	446	GLU	3.1
1	B	450	GLN	3.1
1	D	786	PRO	3.0
1	B	442	PRO	3.0
1	D	488	HIS	3.0
1	B	486	GLU	2.9
1	A	470	LEU	2.9
1	D	462	LEU	2.9
1	C	447	GLU	2.9
1	C	485	ILE	2.8
1	C	482	GLU	2.8
1	A	478	ALA	2.8
1	A	829	ASP	2.8
1	C	486	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	2.8
1	D	467	ILE	2.8
1	D	487	THR	2.8
1	D	515	ARG	2.7
1	C	478	ALA	2.6
1	D	468	ILE	2.6
1	C	860	GLY	2.5
1	C	607	ALA	2.5
1	C	829	ASP	2.5
1	C	515	ARG	2.5
1	A	447	GLU	2.4
1	B	756	ILE	2.4
1	A	789	GLU	2.4
1	D	463	SER	2.4
1	B	524	GLY	2.4
1	C	445	ASN	2.4
1	A	718	ARG	2.3
1	D	630	ARG	2.3
1	A	846	VAL	2.3
1	A	760	ILE	2.3
1	A	475	HIS	2.3
1	B	461	PHE	2.3
1	A	785	GLY	2.3
1	D	472	ASN	2.3
1	C	454	ASN	2.2
1	C	488	HIS	2.2
1	A	756	ILE	2.1
1	A	461	PHE	2.1
1	B	441	GLU	2.1
1	C	448	CYS	2.1
1	D	617	VAL	2.1
1	D	466	GLU	2.1
1	B	718	ARG	2.0
1	C	828	LYS	2.0
1	B	446	GLU	2.0
1	C	469	GLN	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 [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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	3HI	B	1	42/42	0.87	0.14	1.06	22,39,52,53	0
2	3HI	C	4	42/42	0.86	0.14	0.96	23,40,42,44	0
2	3HI	B	2	42/42	0.90	0.14	0.66	23,33,53,54	0
2	3HI	D	3	42/42	0.91	0.13	0.36	21,34,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.