



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:51 AM GMT

PDB ID : 3CD5
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 : 2.39 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

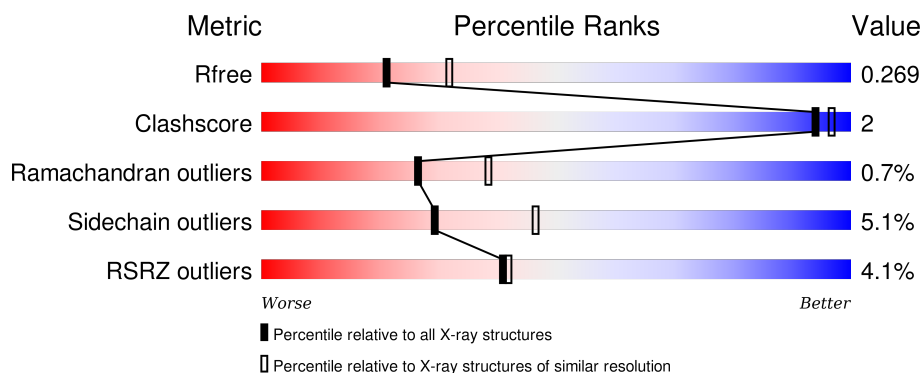
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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 ≥ 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>84% 11% . .</div> </div>
1	B	441	<div> <div>2%</div> <div>87% 9% .</div> </div>
1	C	441	<div> <div>4%</div> <div>88% 7% 5%</div> </div>
1	D	441	<div> <div>6%</div> <div>86% 7% . 6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13170 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	425	Total	C	N	O	S	0	0	0
			3163	1971	556	606	30			
1	B	425	Total	C	N	O	S	0	0	0
			3163	1971	556	606	30			
1	C	418	Total	C	N	O	S	0	4	0
			3126	1947	552	597	30			
1	D	416	Total	C	N	O	S	0	1	0
			3100	1932	546	592	30			

There are 28 discrepancies between the modelled and reference sequences:

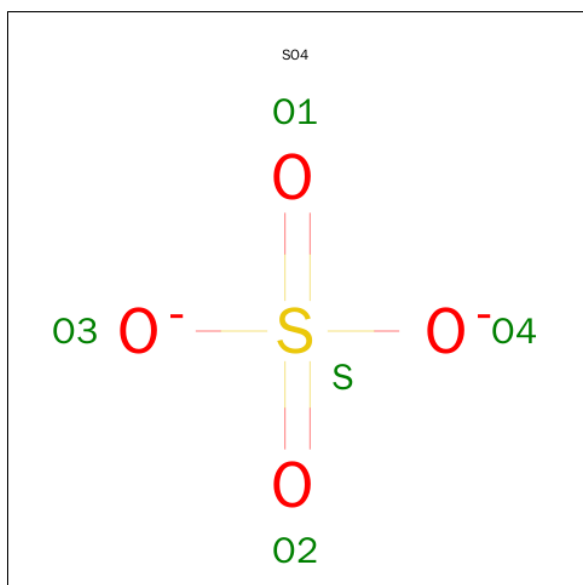
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered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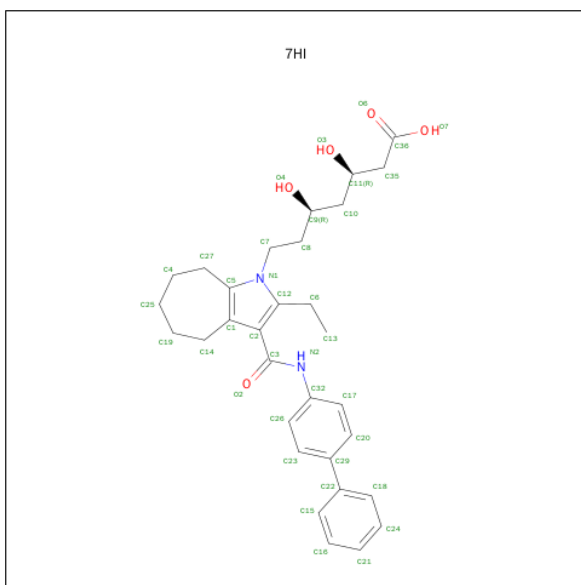
Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (3R,5R)-7-[3-(BIPHENYL-4-YLCARBAMOYL)-2-ETHYL-5,6,7,8-TETRAHYDROCYCLOHEPTA[B]PYRROL-1(4H)-YL]-3,5-DIHYDROXYHEPTANOIC ACID (three-letter code: 7HI) (formula: C₃₁H₃₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 38	C 31	N 2	O 5	0	0
3	B	1	Total 38	C 31	N 2	O 5	0	0
3	D	1	Total 38	C 31	N 2	O 5	0	0
3	D	1	Total 38	C 31	N 2	O 5	0	0

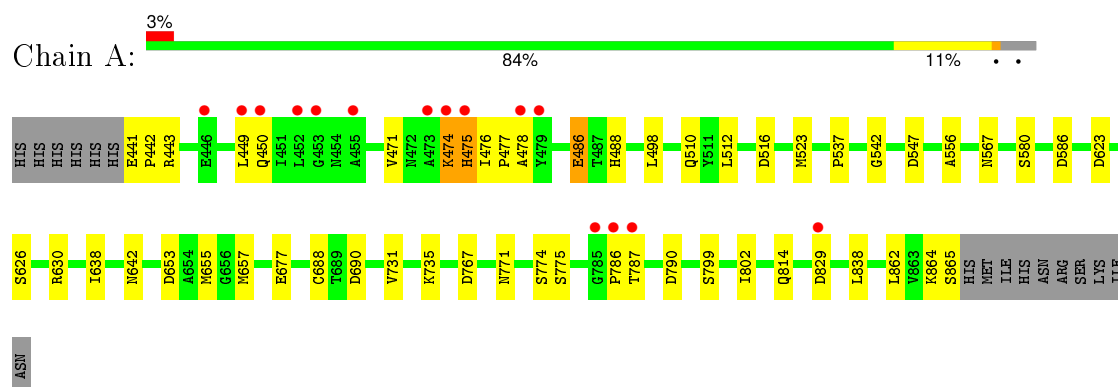
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	128	Total O 128 128	0	0
4	B	118	Total O 118 118	0	0
4	C	98	Total O 98 98	0	0
4	D	102	Total O 102 102	0	0

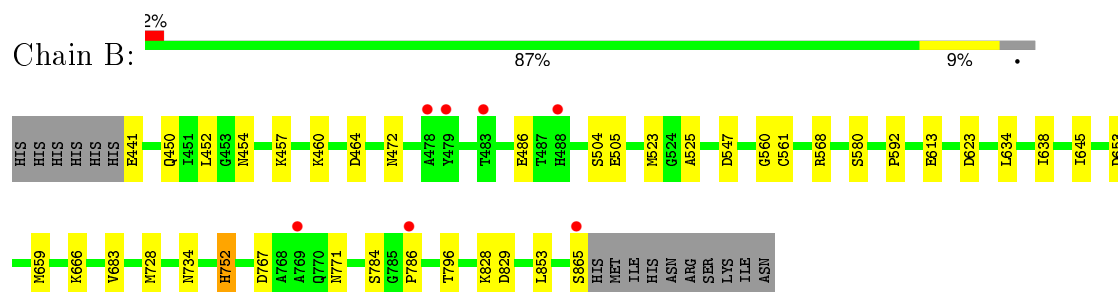
3 Residue-property plots [i](#)

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.

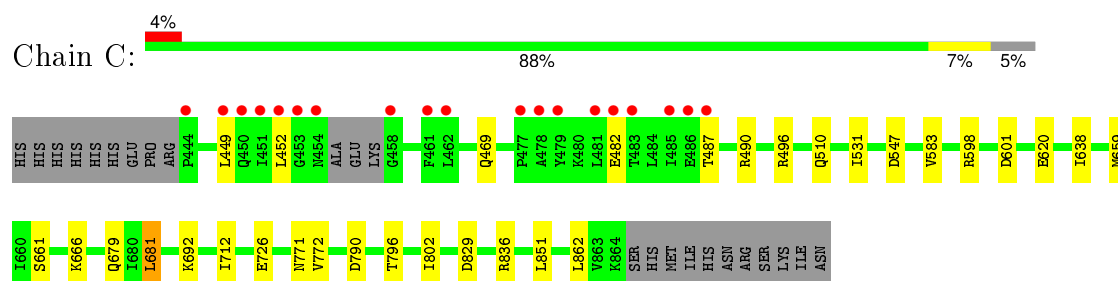
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



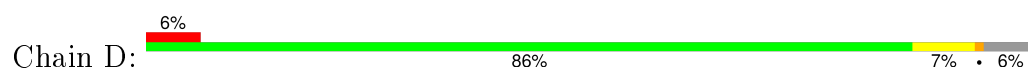
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

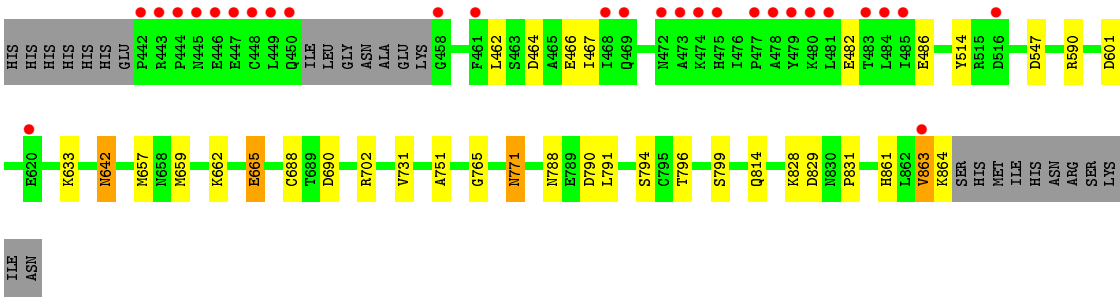


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- 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	73.04Å 173.18Å 75.96Å 90.00° 118.76° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 31.70 – 2.39	Depositor EDS
% Data completeness (in resolution range)	60.8 (50.00-2.39) 60.6 (31.70-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.273 0.199 , 0.269	Depositor DCC
R_{free} test set	2011 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.6	EDS
Estimated twinning fraction	0.004 for l,k,-h-l 0.004 for -h-l,k,h 0.044 for h,-k,-h-l 0.053 for l,-k,h 0.032 for -h-l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39736 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13170	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: 7HI, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/3209	0.62	9/4338 (0.2%)
1	B	0.33	0/3209	0.61	6/4338 (0.1%)
1	C	0.32	0/3190	0.59	4/4309 (0.1%)
1	D	0.33	0/3150	0.62	5/4257 (0.1%)
All	All	0.33	0/12758	0.61	24/17242 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	790	ASP	CB-CG-OD2	6.32	123.98	118.30
1	B	623	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	547	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	547	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	547	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	790	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	516	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	829	ASP	CB-CG-OD2	5.34	123.10	118.30
1	D	690	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	767	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	464	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	653	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	790	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	547	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	767	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	586	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	653	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	829	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	690	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	601	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	829	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	623	ASP	CB-CG-OD2	5.09	122.89	118.30
1	D	464	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	601	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	3163	0	3205	15	0
1	B	3163	0	3205	9	0
1	C	3126	0	3172	11	0
1	D	3100	0	3141	21	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	38	0	37	0	0
3	B	38	0	37	1	0
3	D	76	0	74	4	0
4	A	128	0	0	0	0
4	B	118	0	0	0	0
4	C	98	0	0	0	0
4	D	102	0	0	0	0
All	All	13170	0	12871	47	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 (47) 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:D:863:VAL:HB	1:D:864:LYS:HA	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:VAL:CB	1:D:864:LYS:HA	1.94	0.98
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:OD1	2.10	0.83
1:D:863:VAL:CG2	1:D:864:LYS:HA	2.15	0.76
1:A:441:GLU:N	1:A:442:PRO:CD	2.62	0.63
1:D:863:VAL:HG23	1:D:864:LYS:HA	1.82	0.62
1:D:863:VAL:HB	1:D:864:LYS:CA	2.24	0.61
1:C:771[A]:ASN:ND2	1:D:771[A]:ASN:OD1	2.35	0.57
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.84	0.57
1:A:441:GLU:N	1:A:442:PRO:HD3	2.22	0.55
1:A:731:VAL:O	1:A:735:LYS:HB3	2.07	0.54
3:D:876:7HI:H8A	3:D:876:7HI:H13A	1.90	0.54
1:A:542:GLY:H	1:A:567:ASN:HD22	1.56	0.52
1:D:863:VAL:HG23	1:D:864:LYS:CA	2.39	0.52
1:C:583:VAL:HG11	1:C:836[B]:ARG:HD2	1.93	0.50
1:D:642:ASN:HD22	1:D:642:ASN:N	2.09	0.50
1:D:590:ARG:CZ	1:D:657:MET:HE1	2.43	0.49
1:C:692:LYS:NZ	1:D:751:ALA:O	2.36	0.48
1:B:638:ILE:O	1:C:796:THR:HG21	2.14	0.48
1:D:462:LEU:HD12	1:D:467:ILE:HD11	1.99	0.45
1:C:496:ARG:HD2	1:C:531:ILE:O	2.17	0.45
1:A:774:SER:HA	1:A:799:SER:O	2.17	0.45
1:D:861:HIS:HB3	3:D:3:7HI:H19A	1.99	0.44
1:A:771:ASN:OD1	1:A:775:SER:OG	2.34	0.44
1:B:560:GLY:O	1:B:561:CYS:HB2	2.18	0.43
1:C:712:ILE:HG13	1:C:851:LEU:HD11	1.99	0.43
1:A:542:GLY:H	1:A:567:ASN:ND2	2.16	0.42
1:B:752:HIS:ND1	1:B:853:LEU:HD22	2.35	0.42
1:B:454:ASN:HB3	1:B:457:LYS:HB2	2.01	0.42
1:A:638:ILE:O	1:D:796:THR:HG21	2.20	0.42
3:D:3:7HI:H13A	3:D:3:7HI:H8A	2.02	0.42
1:B:592:PRO:HD2	1:B:645:ILE:O	2.19	0.42
1:B:796:THR:HG21	1:C:638:ILE:O	2.20	0.42
1:A:471:VAL:HA	1:A:476:ILE:O	2.20	0.41
1:C:862:LEU:HB2	1:D:665:GLU:HG3	2.02	0.41
1:D:863:VAL:CG2	3:D:3:7HI:H14A	2.51	0.41
1:D:702:ARG:O	1:D:799:SER:HA	2.19	0.41
1:D:765:GLY:CA	1:D:814:GLN:HG2	2.51	0.41
1:D:863:VAL:HG23	1:D:864:LYS:HB3	2.03	0.41
1:A:862:LEU:HD23	1:B:683:VAL:HB	2.02	0.41
1:A:642:ASN:HD21	1:B:734:ASN:CG	2.23	0.41
1:B:568:ARG:HD3	3:B:1:7HI:C15	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:HIS:CD2	1:A:523:MET:HG3	2.56	0.40
1:C:772:VAL:HG23	1:D:771[B]:ASN:HD21	1.86	0.40
1:A:537:PRO:O	1:A:556:ALA:HA	2.21	0.40
1:A:802:ILE:HG12	1:A:838:LEU:HD23	2.02	0.40
1:A:655:MET:SD	1:A:657:MET:HG2	2.61	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	423/441 (96%)	401 (95%)	16 (4%)	6 (1%)	14	19
1	B	423/441 (96%)	404 (96%)	17 (4%)	2 (0%)	34	48
1	C	418/441 (95%)	401 (96%)	17 (4%)	0	100	100
1	D	413/441 (94%)	391 (95%)	19 (5%)	3 (1%)	26	38
All	All	1677/1764 (95%)	1597 (95%)	69 (4%)	11 (1%)	26	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474	LYS
1	A	478	ALA
1	A	486	GLU
1	B	525	ALA
1	A	786	PRO
1	B	786	PRO
1	A	475	HIS
1	A	477	PRO
1	D	514	TYR
1	D	831	PRO

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Mol	Chain	Res	Type
1	D	863	VAL

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	339/355 (96%)	321 (95%)	18 (5%)	28	44
1	B	339/355 (96%)	319 (94%)	20 (6%)	24	38
1	C	337/355 (95%)	321 (95%)	16 (5%)	32	50
1	D	333/355 (94%)	317 (95%)	16 (5%)	31	49
All	All	1348/1420 (95%)	1278 (95%)	70 (5%)	29	45

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	A	449	LEU
1	A	450	GLN
1	A	474	LYS
1	A	475	HIS
1	A	486	GLU
1	A	498	LEU
1	A	510	GLN
1	A	512	LEU
1	A	580	SER
1	A	626	SER
1	A	630	ARG
1	A	677	GLU
1	A	688	CYS
1	A	787	THR
1	A	814	GLN
1	A	864	LYS
1	A	865	SER
1	B	441	GLU
1	B	450	GLN

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Mol	Chain	Res	Type
1	B	452	LEU
1	B	460	LYS
1	B	472	ASN
1	B	486	GLU
1	B	504	SER
1	B	505	GLU
1	B	523	MET
1	B	580	SER
1	B	613	GLU
1	B	634	LEU
1	B	659	MET
1	B	666	LYS
1	B	728	MET
1	B	752	HIS
1	B	771	ASN
1	B	784	SER
1	B	828	LYS
1	B	865	SER
1	C	449	LEU
1	C	452	LEU
1	C	469	GLN
1	C	482	GLU
1	C	487	THR
1	C	490	ARG
1	C	510	GLN
1	C	598	ARG
1	C	620	GLU
1	C	659	MET
1	C	661	SER
1	C	666	LYS
1	C	679	GLN
1	C	681	LEU
1	C	726	GLU
1	C	802	ILE
1	D	466	GLU
1	D	482	GLU
1	D	486	GLU
1	D	633	LYS
1	D	642	ASN
1	D	659	MET
1	D	662	LYS
1	D	665	GLU

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Mol	Chain	Res	Type
1	D	688	CYS
1	D	771[A]	ASN
1	D	771[B]	ASN
1	D	788	ASN
1	D	791	LEU
1	D	794	SER
1	D	828	LYS
1	D	829	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN
1	A	635	HIS
1	A	788	ASN
1	A	819	GLN
1	B	510	GLN
1	B	529	ASN
1	B	819	GLN
1	C	469	GLN
1	C	472	ASN
1	C	642	ASN
1	C	810	ASN
1	D	472	ASN
1	D	518	ASN
1	D	632	GLN
1	D	642	ASN
1	D	810	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	SO4	A	1	-	4,4,4	0.30	0	6,6,6	0.16	0
3	7HI	A	2	-	36,41,41	1.01	2 (5%)	42,56,56	1.72	7 (16%)
3	7HI	B	1	-	36,41,41	1.02	2 (5%)	42,56,56	1.73	10 (23%)
2	SO4	B	2	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	C	3	-	4,4,4	0.22	0	6,6,6	0.18	0
3	7HI	D	3	-	36,41,41	1.03	3 (8%)	42,56,56	1.99	9 (21%)
2	SO4	D	4	-	4,4,4	0.27	0	6,6,6	0.16	0
3	7HI	D	876	-	36,41,41	0.99	2 (5%)	42,56,56	1.71	9 (21%)

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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
3	7HI	A	2	-	-	0/21/35/35	1/4/4/4
3	7HI	B	1	-	-	0/21/35/35	1/4/4/4
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0
3	7HI	D	3	-	-	0/21/35/35	0/4/4/4
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0
3	7HI	D	876	-	-	0/21/35/35	1/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	7HI	C25-C19	-4.31	1.33	1.51
3	A	2	7HI	C25-C19	-4.30	1.33	1.51
3	B	1	7HI	C25-C19	-4.28	1.33	1.51
3	D	876	7HI	C25-C19	-4.25	1.33	1.51
3	B	1	7HI	C32-N2	-2.80	1.36	1.41
3	D	876	7HI	C32-N2	-2.61	1.36	1.41
3	A	2	7HI	C32-N2	-2.60	1.36	1.41
3	D	3	7HI	C32-N2	-2.45	1.37	1.41
3	D	3	7HI	C5-C1	2.25	1.40	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	7HI	C8-C7-N1	-6.47	106.83	112.29
3	A	2	7HI	C8-C7-N1	-5.78	107.42	112.29
3	B	1	7HI	C8-C7-N1	-5.47	107.67	112.29
3	D	876	7HI	C8-C7-N1	-4.40	108.58	112.29
3	D	876	7HI	O2-C3-C2	-3.12	116.28	120.80
3	D	3	7HI	C25-C4-C27	-2.99	109.57	114.35
3	D	3	7HI	C10-C11-C35	-2.92	107.37	112.94
3	D	3	7HI	C6-C12-C2	-2.64	125.95	130.41
3	B	1	7HI	C10-C11-C35	-2.64	107.90	112.94
3	D	3	7HI	O2-C3-C2	-2.62	116.99	120.80
3	B	1	7HI	O2-C3-C2	-2.60	117.03	120.80
3	B	1	7HI	C6-C12-C2	-2.44	126.28	130.41
3	A	2	7HI	C6-C12-C2	-2.42	126.33	130.41
3	D	876	7HI	C19-C14-C1	-2.37	109.92	113.92
3	B	1	7HI	C25-C4-C27	-2.32	110.64	114.35
3	A	2	7HI	O2-C3-C2	-2.28	117.50	120.80
3	D	876	7HI	C25-C4-C27	-2.23	110.78	114.35
3	B	1	7HI	C19-C14-C1	-2.20	110.20	113.92
3	D	876	7HI	C6-C12-C2	-2.18	126.72	130.41
3	A	2	7HI	C19-C14-C1	-2.18	110.23	113.92
3	D	3	7HI	C2-C3-N2	2.11	118.99	114.88
3	D	876	7HI	C2-C3-N2	2.38	119.53	114.88
3	B	1	7HI	C2-C3-N2	2.46	119.67	114.88
3	D	876	7HI	C6-C12-N1	2.77	126.56	120.20
3	B	1	7HI	C6-C12-N1	3.03	127.15	120.20
3	A	2	7HI	C6-C12-N1	3.11	127.32	120.20
3	D	3	7HI	C6-C12-N1	3.25	127.64	120.20
3	B	1	7HI	C25-C19-C14	4.33	121.28	114.35
3	A	2	7HI	C25-C19-C14	4.37	121.35	114.35
3	D	876	7HI	C12-C2-C1	4.57	109.70	103.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	7HI	C12-C2-C1	4.57	109.70	103.87
3	D	876	7HI	C25-C19-C14	4.63	121.76	114.35
3	A	2	7HI	C12-C2-C1	4.70	109.87	103.87
3	D	3	7HI	C12-C2-C1	4.95	110.18	103.87
3	D	3	7HI	C25-C19-C14	6.05	124.04	114.35

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	876	7HI	C1-C14-C19-C25-C27-C4-C5
3	A	2	7HI	C1-C14-C19-C25-C27-C4-C5
3	B	1	7HI	C1-C14-C19-C25-C27-C4-C5

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	7HI	1	0
3	D	3	7HI	3	0
3	D	876	7HI	1	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	425/441 (96%)	0.02	15 (3%) 48 48	26, 39, 62, 70	0
1	B	425/441 (96%)	-0.12	7 (1%) 74 74	26, 38, 66, 72	0
1	C	418/441 (94%)	0.01	19 (4%) 37 38	25, 39, 74, 80	0
1	D	416/441 (94%)	0.18	28 (6%) 21 21	26, 40, 71, 76	0
All	All	1684/1764 (95%)	0.02	69 (4%) 41 42	25, 39, 68, 80	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	473	ALA	11.5
1	D	484	LEU	5.6
1	D	478	ALA	5.3
1	C	479	TYR	5.1
1	D	479	TYR	5.0
1	D	472	ASN	4.9
1	D	474	LYS	4.8
1	C	483	THR	4.7
1	D	446	GLU	4.7
1	D	469	GLN	4.6
1	D	477	PRO	4.5
1	A	479	TYR	4.3
1	C	451	ILE	4.2
1	D	481	LEU	4.2
1	C	461	PHE	4.0
1	C	452	LEU	4.0
1	D	480	LYS	3.7
1	C	450	GLN	3.6
1	C	481	LEU	3.5
1	C	477	PRO	3.4
1	D	450	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	452	LEU	3.4
1	D	443	ARG	3.3
1	C	453	GLY	3.3
1	A	475	HIS	3.3
1	A	473	ALA	3.3
1	D	475	HIS	3.3
1	D	461	PHE	3.0
1	D	483	THR	3.0
1	C	444	PRO	3.0
1	D	448	CYS	3.0
1	D	449	LEU	3.0
1	A	786	PRO	2.9
1	B	786	PRO	2.9
1	A	455	ALA	2.9
1	C	449	LEU	2.9
1	B	479	TYR	2.9
1	A	453	GLY	2.9
1	D	468	ILE	2.9
1	A	450	GLN	2.9
1	B	483	THR	2.8
1	D	447	GLU	2.8
1	A	474	LYS	2.7
1	C	458	GLY	2.7
1	A	829	ASP	2.7
1	C	478	ALA	2.6
1	A	787	THR	2.6
1	D	445	ASN	2.6
1	D	458	GLY	2.6
1	A	446	GLU	2.6
1	C	462	LEU	2.5
1	D	620	GLU	2.5
1	A	478	ALA	2.5
1	C	482	GLU	2.4
1	D	444	PRO	2.4
1	B	488	HIS	2.4
1	B	865	SER	2.3
1	C	485	ILE	2.3
1	D	485	ILE	2.3
1	D	442	PRO	2.3
1	C	454	ASN	2.2
1	D	516	ASP	2.1
1	D	863	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	769	ALA	2.1
1	A	785	GLY	2.1
1	A	449	LEU	2.1
1	B	478	ALA	2.0
1	C	487	THR	2.0
1	C	486	GLU	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, 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(Å ²)	Q<0.9
2	SO4	C	3	5/5	0.94	0.14	0.42	64,64,65,65	0
3	7HI	D	876	38/38	0.92	0.12	-0.02	29,38,39,39	0
3	7HI	D	3	38/38	0.92	0.14	-0.06	28,34,42,42	0
3	7HI	B	1	38/38	0.95	0.12	-0.09	27,32,44,44	0
3	7HI	A	2	38/38	0.93	0.12	-0.36	28,35,54,54	0
2	SO4	A	1	5/5	0.97	0.09	-0.52	59,60,60,60	0
2	SO4	B	2	5/5	0.98	0.09	-0.61	55,55,55,56	0
2	SO4	D	4	5/5	0.97	0.10	-0.77	56,56,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.