Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:15 PM GMT

PDB ID : 3CCZ

Title : Thermodynamic and structure guided design of statin hmg-coa reductase inhibitors

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Deposited on : 2008-02-26

Resolution : 1.70 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

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

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 1.70 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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		2.6%
RSRZ outliers		12.8%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
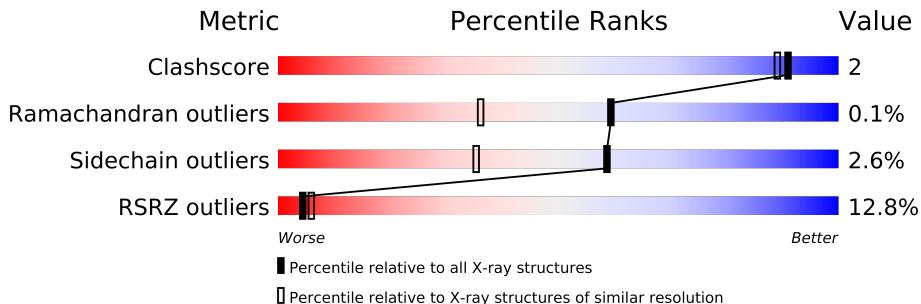
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	
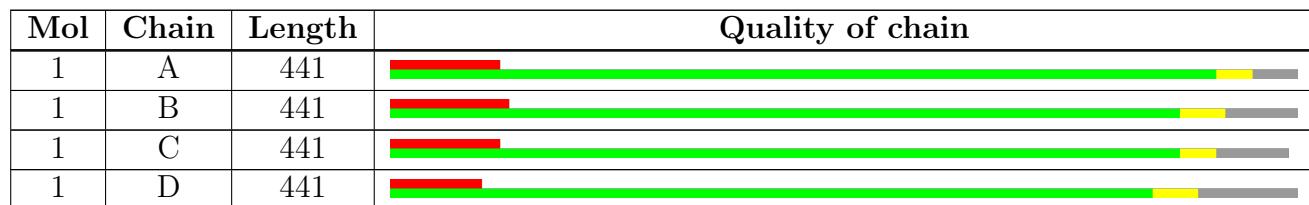
The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1	-	X
2	SO4	B	2	-	X
2	SO4	C	3	-	X
2	SO4	D	4	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13469 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	420	Total 3128	C 1946	N 549	O 601	S 32	0	3	0
1	B	405	Total 3014	C 1874	N 529	O 580	S 31	0	3	0
1	C	404	Total 2997	C 1862	N 524	O 579	S 32	0	3	0
1	D	394	Total 2922	C 1815	N 512	O 565	S 30	0	4	0

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: O_4S).
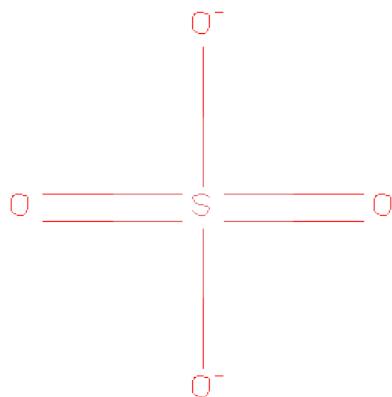
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

• Molecule 3 is (3R,5R)-7-[2-(4-FLUOROPHENYL)-4-{[(1S)-2-HYDROXY-1-PHENYLETH YL]CARBAMOYL}-5-(1-METHYLETHYL)-1H-IMIDAZOL-1-YL]-3,5-DIHYDROXYHEP TANOICACID (three-letter code: 5HI) (formula: $C_{28}H_{34}FN_3O_6$).
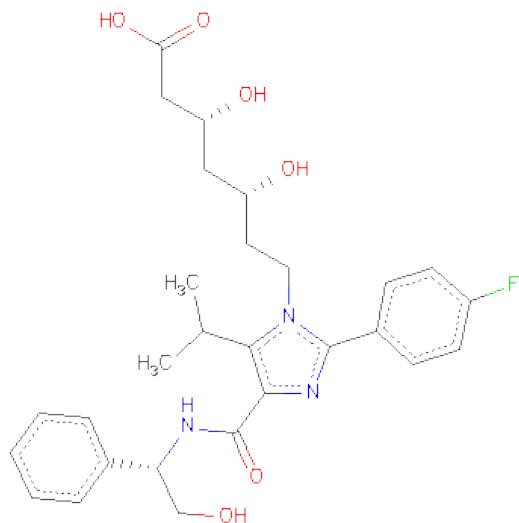
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
3	B	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
3	C	1	Total	C	F	N	O	0	0
			38	28	1	3	6		
3	D	1	Total	C	F	N	O	0	0
			38	28	1	3	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total	O	0	0
			335	335		
4	B	316	Total	O	0	0
			316	316		
4	C	293	Total	O	0	0
			293	293		
4	D	292	Total	O	0	0
			292	292		

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
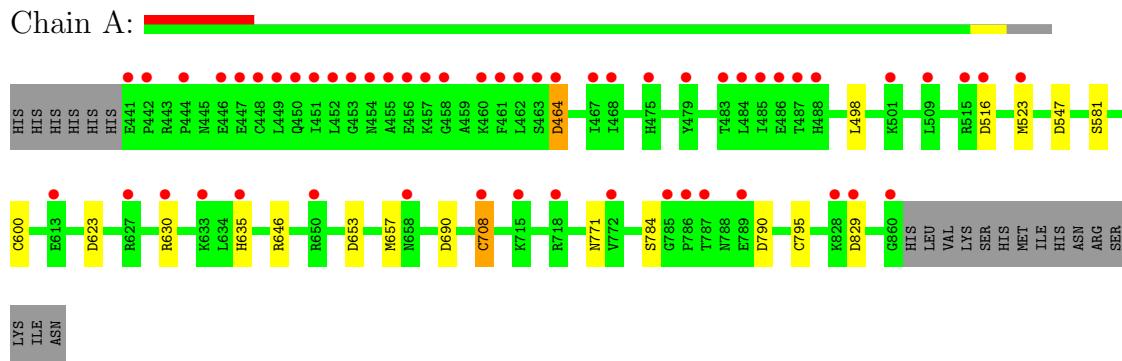
Chain A:

• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase
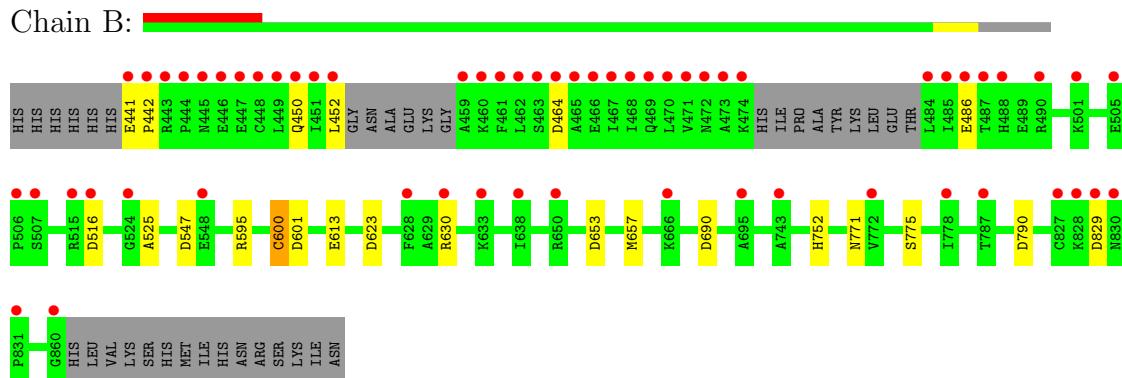
Chain B:

• Molecule 1: 3-hydroxy-3-methylglutaryl-coenzymeA reductase
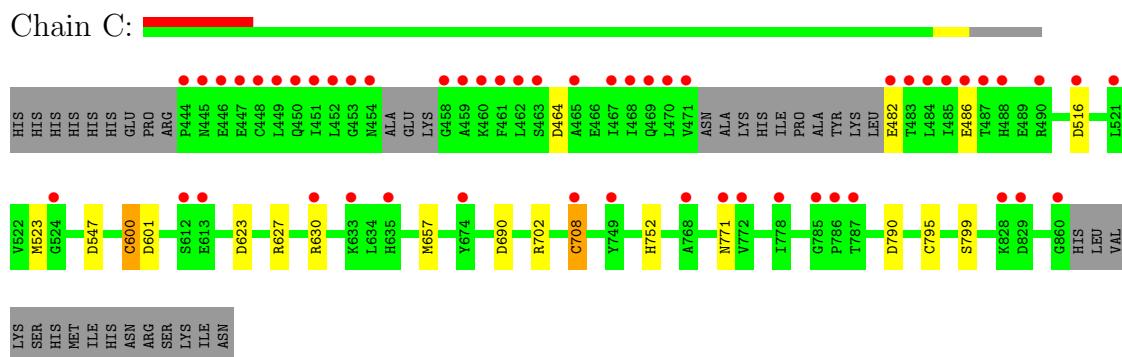
Chain C:

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

Chain D:
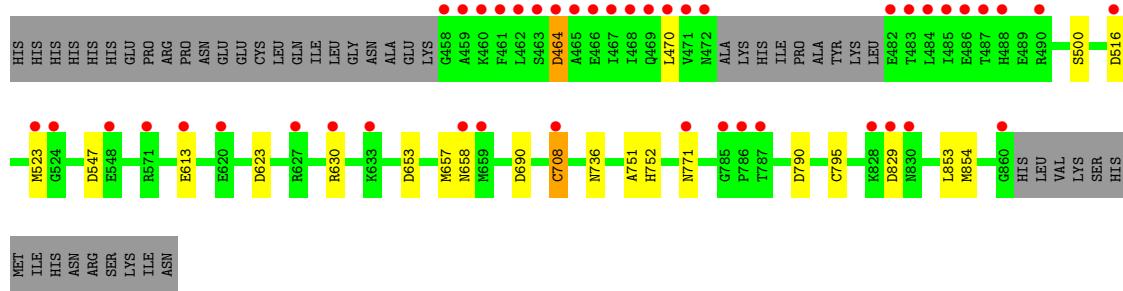
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.86Å 135.66Å 83.15Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 41.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-1.70) 91.0 (41.11-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.03 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.257 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 39.6	EDS
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 186805 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13469	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 5HI

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	0.26	0/3188	0.57	10/4310 (0.2%)
1	B	0.26	0/3069	0.56	10/4146 (0.2%)
1	C	0.25	0/3051	0.57	8/4121 (0.2%)
1	D	0.26	0/2981	0.57	8/4028 (0.2%)
All	All	0.26	0/12289	0.57	36/16605 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	547	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	547	ASP	CB-CG-OD2	5.62	123.35	118.30
1	C	547	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	547	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	790	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	790	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	600[A]	CYS	CA-CB-SG	-5.35	104.37	114.00
1	A	600[B]	CYS	CA-CB-SG	-5.35	104.37	114.00
1	B	790	ASP	CB-CG-OD2	5.34	123.10	118.30
1	C	790	ASP	CB-CG-OD2	5.33	123.09	118.30
1	D	623	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	600[A]	CYS	CA-CB-SG	-5.32	104.43	114.00
1	C	600[B]	CYS	CA-CB-SG	-5.32	104.43	114.00
1	A	653	ASP	CB-CG-OD2	5.28	123.06	118.30
1	C	516	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	516	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	690	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	623	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	623	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	829	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	600[A]	CYS	CA-CB-SG	-5.21	104.63	114.00
1	B	600[B]	CYS	CA-CB-SG	-5.21	104.63	114.00
1	B	690	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	653	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	464	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	516	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	829	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	829	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	464	ASP	CB-CG-OD2	5.09	122.89	118.30
1	D	653	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	690	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	464	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	464	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	516	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	623	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	690	ASP	CB-CG-OD2	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts (i)

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	3128	0	3164	22	0
1	B	3014	0	3050	22	0
1	C	2997	0	3026	16	0
1	D	2922	0	2953	19	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	33	0	0
3	B	38	0	33	1	0
3	C	38	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	38	0	33	0	0
4	A	335	0	0	0	0
4	B	316	0	0	0	0
4	C	293	0	0	0	0
4	D	292	0	0	0	0
All	All	13469	0	12325	49	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 (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:771[B]:ASN:OD1	1:B:771[B]:ASN:ND2	1.69	1.25
1:C:771[B]:ASN:HD21	1:D:771[B]:ASN:CG	1.44	1.21
1:A:771[B]:ASN:ND2	1:B:771[B]:ASN:OD1	1.75	1.17
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:OD1	1.76	1.16
1:A:771[B]:ASN:CG	1:B:771[B]:ASN:HD21	1.68	0.95
1:C:771[B]:ASN:HD21	1:D:771[B]:ASN:ND2	1.64	0.95
1:A:771[B]:ASN:HD21	1:B:771[B]:ASN:CG	1.72	0.93
1:C:771[B]:ASN:CG	1:D:771[B]:ASN:HD21	1.72	0.91
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:CG	2.26	0.85
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:ND2	2.24	0.85
1:C:771[B]:ASN:ND2	1:D:771[B]:ASN:HD21	1.76	0.84
1:C:771[A]:ASN:OD1	1:D:771[A]:ASN:ND2	2.09	0.84
1:C:771[A]:ASN:OD1	1:D:771[A]:ASN:OD1	2.03	0.77
1:D:751:ALA:HB2	1:D:854:MET:CE	2.20	0.71
1:A:771[A]:ASN:HD21	1:B:771[A]:ASN:CG	1.95	0.69
1:C:771[A]:ASN:OD1	1:D:771[A]:ASN:CG	2.32	0.68
1:A:771[A]:ASN:CG	1:B:771[A]:ASN:HD21	1.97	0.67
1:A:771[A]:ASN:OD1	1:B:771[A]:ASN:OD1	2.13	0.67
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:ND2	2.46	0.64
1:D:751:ALA:HB2	1:D:854:MET:HE2	1.80	0.62
1:C:771[B]:ASN:OD1	1:D:771[B]:ASN:ND2	2.28	0.59
1:A:771[A]:ASN:HD21	1:B:771[A]:ASN:ND2	2.00	0.59
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:OD1	2.35	0.59
1:D:751:ALA:HB2	1:D:854:MET:HE3	1.84	0.58
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:HD21	2.01	0.57
1:A:771[A]:ASN:OD1	1:B:771[A]:ASN:ND2	2.36	0.57
1:C:708[B]:CYS:SG	1:C:795:CYS:HB2	2.47	0.54
1:C:771[A]:ASN:ND2	1:D:771[A]:ASN:OD1	2.43	0.52
1:D:708[B]:CYS:SG	1:D:795:CYS:HB2	2.49	0.52
1:A:771[B]:ASN:CG	1:B:771[B]:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:771[A]:ASN:CG	1:B:771[A]:ASN:OD1	2.49	0.51
1:A:771[A]:ASN:CG	1:B:771[A]:ASN:ND2	2.64	0.50
1:A:771[A]:ASN:ND2	1:B:771[A]:ASN:CG	2.63	0.49
1:A:771[B]:ASN:ND2	1:B:771[B]:ASN:CG	2.47	0.49
1:A:771[A]:ASN:OD1	1:B:771[A]:ASN:CG	2.50	0.48
1:A:635:HIS:HB3	1:A:646:ARG:HB3	1.95	0.47
1:A:771[B]:ASN:ND2	1:B:771[B]:ASN:ND2	2.62	0.47
1:D:736:ASN:HD21	1:D:854:MET:HE3	1.79	0.47
3:B:876:5HI:O2	3:B:876:5HI:H13A	2.15	0.47
1:C:771[A]:ASN:CG	1:D:771[A]:ASN:OD1	2.53	0.46
1:D:751:ALA:HB1	1:D:853:LEU:HD23	1.96	0.46
1:A:708[B]:CYS:SG	1:A:795:CYS:HB2	2.57	0.44
1:C:702:ARG:O	1:C:799:SER:HA	2.18	0.44
1:B:600[B]:CYS:SG	1:B:601:ASP:N	2.92	0.43
3:C:876:5HI:O2	3:C:876:5HI:H12A	2.17	0.43
1:A:581:SER:HB3	1:A:708[A]:CYS:SG	2.58	0.43
1:B:441:GLU:N	1:B:442:PRO:CD	2.83	0.42
1:C:600[B]:CYS:SG	1:C:601:ASP:N	2.95	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	421/441 (96%)	405 (96%)	16 (4%)	0	100	100
1	B	402/441 (91%)	390 (97%)	11 (3%)	1 (0%)	56	33
1	C	401/441 (91%)	387 (96%)	14 (4%)	0	100	100
1	D	394/441 (89%)	382 (97%)	12 (3%)	0	100	100
All	All	1618/1764 (92%)	1564 (97%)	53 (3%)	1 (0%)	59	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	337/355 (95%)	329 (98%)	8 (2%)	61	39
1	B	326/355 (92%)	318 (98%)	8 (2%)	60	37
1	C	324/355 (91%)	315 (97%)	9 (3%)	56	32
1	D	316/355 (89%)	304 (96%)	12 (4%)	44	19
All	All	1303/1420 (92%)	1266 (97%)	37 (3%)	59	32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	ASP
1	A	498	LEU
1	A	523	MET
1	A	630	ARG
1	A	657	MET
1	A	708[A]	CYS
1	A	708[B]	CYS
1	A	784	SER
1	B	450	GLN
1	B	452	LEU
1	B	486	GLU
1	B	595	ARG
1	B	613	GLU
1	B	630	ARG
1	B	657	MET
1	B	752	HIS
1	C	482	GLU
1	C	486	GLU
1	C	523	MET
1	C	627	ARG
1	C	630	ARG
1	C	657	MET

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Mol	Chain	Res	Type
1	C	708[A]	CYS
1	C	708[B]	CYS
1	C	752	HIS
1	D	464	ASP
1	D	470	LEU
1	D	500[A]	SER
1	D	500[B]	SER
1	D	523	MET
1	D	613	GLU
1	D	630	ARG
1	D	657	MET
1	D	658	ASN
1	D	708[A]	CYS
1	D	708[B]	CYS
1	D	752	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	819	GLN
1	B	819	GLN
1	C	632	GLN
1	C	819	GLN

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 ⓘ

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	0.23	0	6,6,6	0.08	0
3	5HI	A	876	-	40,40,40	0.70	0	55,55,55	1.31	6 (10%)
2	SO4	B	2	-	4,4,4	0.22	0	6,6,6	0.07	0
3	5HI	B	876	-	40,40,40	0.70	0	55,55,55	1.46	6 (10%)
2	SO4	C	3	-	4,4,4	0.24	0	6,6,6	0.09	0
3	5HI	C	876	-	40,40,40	0.71	0	55,55,55	1.40	7 (12%)
2	SO4	D	4	-	4,4,4	0.24	0	6,6,6	0.07	0
3	5HI	D	876	-	40,40,40	0.71	0	55,55,55	1.45	6 (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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
3	5HI	A	876	-	-	0/33/35/35	0/3/3/3
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0
3	5HI	B	876	-	-	0/33/35/35	0/3/3/3
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0
3	5HI	C	876	-	-	0/33/35/35	0/3/3/3
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0
3	5HI	D	876	-	-	0/33/35/35	0/3/3/3

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	876	5HI	C8-C7-N1	-5.64	107.72	112.31
3	D	876	5HI	C8-C7-N1	-5.52	107.82	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	876	5HI	C8-C7-N1	-5.41	107.91	112.31
3	D	876	5HI	C14-C1-N2	-4.68	103.66	109.56
3	A	876	5HI	C8-C7-N1	-4.45	108.69	112.31
3	C	876	5HI	C14-C1-N2	-3.51	105.13	109.56
3	B	876	5HI	C14-C1-N2	-3.49	105.15	109.56
3	B	876	5HI	C7-C8-C9	3.03	116.69	113.82
3	A	876	5HI	C14-C1-N2	-2.98	105.81	109.56
3	B	876	5HI	C2-C3-N2	2.74	118.67	115.92
3	A	876	5HI	C27-C5-N1	2.50	128.25	124.76
3	C	876	5HI	C27-C5-N1	2.28	127.94	124.76
3	C	876	5HI	C2-C3-N2	2.25	118.17	115.92
3	C	876	5HI	C19-C2-C3	-2.24	126.46	130.70
3	B	876	5HI	C27-C5-N1	2.23	127.88	124.76
3	A	876	5HI	C32-C1-N2	2.22	116.55	111.81
3	C	876	5HI	C24-C30-C15	-2.18	119.93	122.90
3	B	876	5HI	C24-C30-C15	-2.17	119.95	122.90
3	A	876	5HI	C1-N2-C3	2.14	125.63	122.41
3	D	876	5HI	C24-C30-C15	-2.13	120.00	122.90
3	D	876	5HI	C32-C1-N2	2.12	116.34	111.81
3	D	876	5HI	C27-C5-N1	2.09	127.67	124.76
3	C	876	5HI	C32-C1-N2	2.05	116.19	111.81
3	A	876	5HI	C24-C30-C15	-2.05	120.12	122.90
3	D	876	5HI	C19-C2-C3	-2.02	126.87	130.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7   Other polymers (i)

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	420/441 (95%)	0.96	54 (12%)	4	6	15, 24, 54, 79	0
1	B	405/441 (91%)	1.04	59 (14%)	3	4	14, 24, 80, 99	0
1	C	404/441 (91%)	1.12	52 (12%)	4	6	14, 23, 80, 96	0
1	D	394/441 (89%)	0.94	44 (11%)	6	8	14, 24, 59, 93	0
All	All	1623/1764 (92%)	1.01	209 (12%)	4	6	14, 23, 69, 99	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	484	LEU	12.3
1	B	461	PHE	12.2
1	D	458	GLY	11.7
1	A	453	GLY	11.4
1	C	461	PHE	10.8
1	C	483	THR	10.6
1	B	474	LYS	10.6
1	C	453	GLY	10.5
1	B	450	GLN	10.4
1	B	449	LEU	10.2
1	D	461	PHE	10.2
1	C	484	LEU	10.2
1	D	470	LEU	10.1
1	D	469	GLN	9.7
1	C	449	LEU	9.5
1	D	462	LEU	9.4
1	D	472	ASN	9.3
1	A	455	ALA	9.1
1	B	452	LEU	8.8
1	D	483	THR	8.7
1	C	444	PRO	8.6

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Mol	Chain	Res	Type	RSRZ
1	C	458	GLY	8.0
1	C	471	VAL	7.8
1	B	451	ILE	7.7
1	C	452	LEU	7.7
1	B	444	PRO	7.1
1	A	452	LEU	7.0
1	A	461	PHE	7.0
1	C	451	ILE	7.0
1	D	468	ILE	6.9
1	C	454	ASN	6.9
1	B	442	PRO	6.9
1	C	462	LEU	6.8
1	D	471	VAL	6.8
1	C	469	GLN	6.8
1	A	441	GLU	6.8
1	C	487	THR	6.7
1	B	441	GLU	6.6
1	D	486	GLU	6.6
1	C	486	GLU	6.6
1	C	448	CYS	6.3
1	A	442	PRO	6.2
1	B	462	LEU	6.1
1	C	446	GLU	6.0
1	C	450	GLN	5.9
1	D	459	ALA	5.9
1	C	470	LEU	5.8
1	A	450	GLN	5.8
1	C	482	GLU	5.6
1	B	471	VAL	5.6
1	A	456	GLU	5.5
1	B	484	LEU	5.5
1	B	448	CYS	5.4
1	A	454	ASN	5.3
1	B	473	ALA	5.3
1	D	467	ILE	5.2
1	C	447	GLU	5.2
1	D	485	ILE	5.0
1	D	487	THR	4.9
1	A	458	GLY	4.7
1	A	635	HIS	4.6
1	A	457	LYS	4.4
1	B	446	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	445	ASN	4.4
1	A	446	GLU	4.4
1	A	786	PRO	4.3
1	A	828	LYS	4.2
1	C	708[A]	CYS	4.2
1	C	829	ASP	4.2
1	B	488	HIS	4.2
1	C	860	GLY	4.1
1	B	828	LYS	4.1
1	C	460	LYS	4.1
1	A	444	PRO	4.1
1	A	484	LEU	4.1
1	A	462	LEU	4.0
1	D	786	PRO	4.0
1	C	786	PRO	4.0
1	B	468	ILE	4.0
1	D	460	LYS	3.9
1	D	465	ALA	3.8
1	B	445	ASN	3.8
1	B	447	GLU	3.7
1	B	460	LYS	3.7
1	C	488	HIS	3.7
1	C	828	LYS	3.7
1	B	486	GLU	3.6
1	A	787	THR	3.6
1	A	785	GLY	3.6
1	B	465	ALA	3.6
1	A	483	THR	3.6
1	B	470	LEU	3.5
1	A	449	LEU	3.5
1	C	785	GLY	3.5
1	A	630	ARG	3.5
1	B	463	SER	3.5
1	A	860	GLY	3.4
1	C	787	THR	3.4
1	B	633	LYS	3.4
1	B	829	ASP	3.4
1	B	485	ILE	3.4
1	C	485	ILE	3.4
1	D	829	ASP	3.3
1	B	487	THR	3.3
1	B	516	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	459	ALA	3.3
1	A	708[A]	CYS	3.3
1	D	630	ARG	3.2
1	D	482	GLU	3.2
1	A	451	ILE	3.1
1	C	630	ARG	3.1
1	B	459	ALA	3.1
1	D	633	LYS	3.1
1	D	708[A]	CYS	3.1
1	A	485	ILE	3.1
1	A	475	HIS	3.0
1	D	828	LYS	3.0
1	C	490	ARG	3.0
1	C	468	ILE	3.0
1	D	466	GLU	2.9
1	A	633	LYS	2.9
1	B	466	GLU	2.9
1	D	627	ARG	2.9
1	A	829	ASP	2.9
1	B	506	PRO	2.9
1	C	465	ALA	2.8
1	A	448	CYS	2.8
1	B	772	VAL	2.7
1	B	501	LYS	2.7
1	D	860	GLY	2.7
1	C	463	SER	2.7
1	D	490	ARG	2.7
1	D	613	GLU	2.7
1	A	460	LYS	2.7
1	B	464	ASP	2.6
1	A	789	GLU	2.6
1	D	524	GLY	2.6
1	A	718	ARG	2.6
1	C	612	SER	2.6
1	B	743	ALA	2.5
1	A	523	MET	2.5
1	B	515	ARG	2.5
1	A	516	ASP	2.5
1	C	771[A]	ASN	2.5
1	D	548	GLU	2.5
1	B	860	GLY	2.5
1	C	613	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	620	GLU	2.4
1	A	447	GLU	2.4
1	A	772	VAL	2.4
1	D	830	ASN	2.4
1	D	464	ASP	2.4
1	A	515	ARG	2.4
1	A	488	HIS	2.4
1	B	831	PRO	2.4
1	A	487	THR	2.4
1	D	463	SER	2.4
1	A	650	ARG	2.4
1	D	787	THR	2.4
1	A	479	TYR	2.4
1	D	659	MET	2.4
1	B	490	ARG	2.3
1	A	463	SER	2.3
1	D	523	MET	2.3
1	C	772	VAL	2.3
1	D	516	ASP	2.3
1	D	488	HIS	2.3
1	B	467	ILE	2.2
1	B	472	ASN	2.2
1	D	771[A]	ASN	2.2
1	B	469	GLN	2.2
1	D	658	ASN	2.2
1	B	695	ALA	2.2
1	C	633	LYS	2.2
1	A	464	ASP	2.2
1	C	467	ILE	2.2
1	D	785	GLY	2.2
1	A	467	ILE	2.2
1	C	778	ILE	2.2
1	B	443	ARG	2.2
1	B	666	LYS	2.2
1	D	571	ARG	2.2
1	C	768	ALA	2.2
1	A	658	ASN	2.2
1	A	509	LEU	2.1
1	C	521	LEU	2.1
1	B	548	GLU	2.1
1	A	468	ILE	2.1
1	C	516	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	507	SER	2.1
1	A	501	LYS	2.1
1	B	524	GLY	2.1
1	B	628	PHE	2.1
1	B	827	CYS	2.1
1	B	830	ASN	2.1
1	B	787	THR	2.1
1	B	638	ILE	2.1
1	C	524	GLY	2.1
1	A	613	GLU	2.1
1	B	505	GLU	2.1
1	B	630	ARG	2.1
1	A	715	LYS	2.1
1	C	674	TYR	2.0
1	B	650	ARG	2.0
1	A	627	ARG	2.0
1	C	635	HIS	2.0
1	C	749	TYR	2.0
1	B	778	ILE	2.0
1	A	486	GLU	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(Å^2)	Q<0.9
2	SO4	B	2	5/5	0.25	4.61	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
2	SO4	C	3	5/5	0.27	3.64	70,70,70,70	0
2	SO4	A	1	5/5	0.27	3.26	77,77,77,77	0
2	SO4	D	4	5/5	0.24	2.50	69,69,69,69	0
3	5HI	B	876	38/38	0.14	1.35	21,29,30,30	0
3	5HI	A	876	38/38	0.15	0.80	19,25,27,29	0
3	5HI	D	876	38/38	0.13	0.76	21,27,28,29	0
3	5HI	C	876	38/38	0.13	0.63	20,27,29,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.