Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:50 AM GMT

PDB ID	:	3CCZ
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	:	1.70 Å(reported)

The following versions of software and data (see references (i)) 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
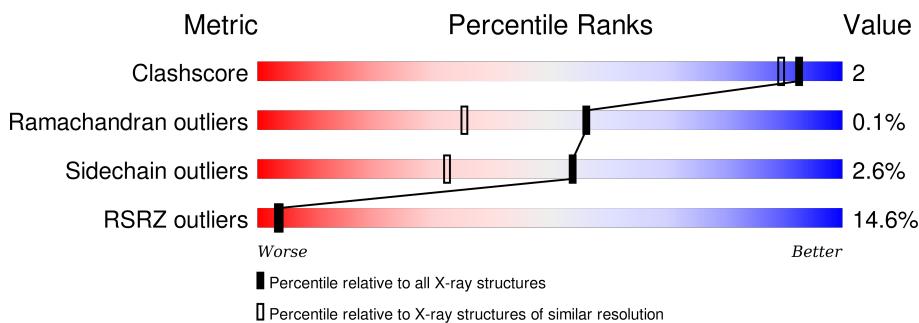
1　Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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		14.6%

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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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. 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 <=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	14% / 91% / · 5%
1	B	441	15% / 87% / 5% 8%
1	C	441	14% / 87% / · 8%
1	D	441	11% / 84% / 5% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 (i)

There are 4 unique types of molecules in this entry. The entry contains 13469 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	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:
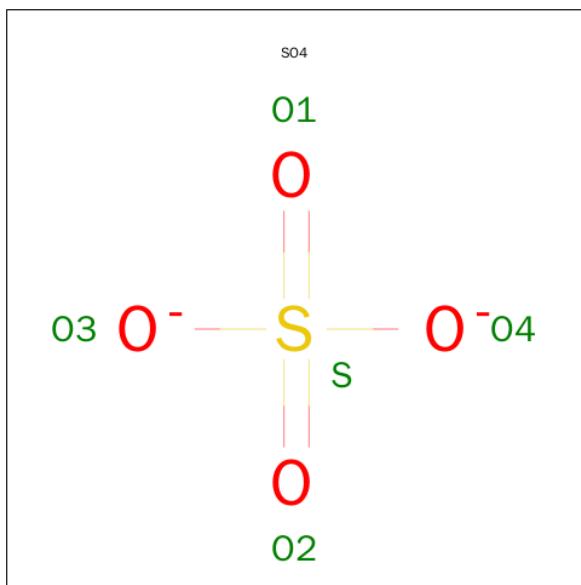
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered	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

Continued on next page...

Continued from previous page...
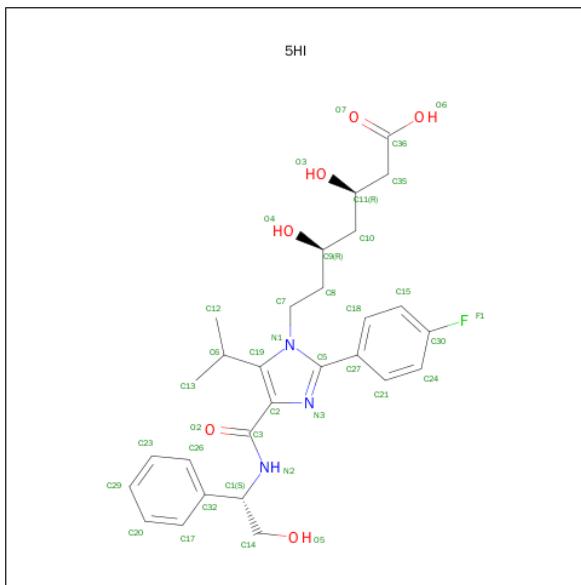
Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered	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 TANOIC ACID (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		
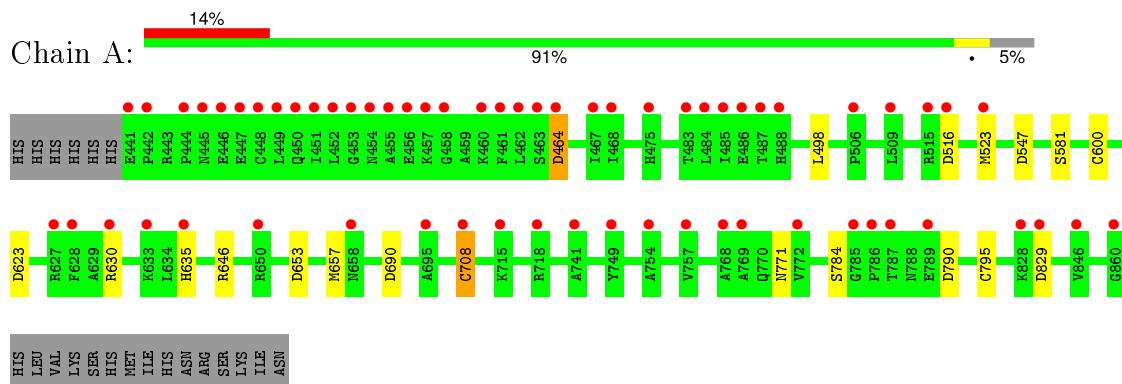
- Molecule 4 is water.

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		
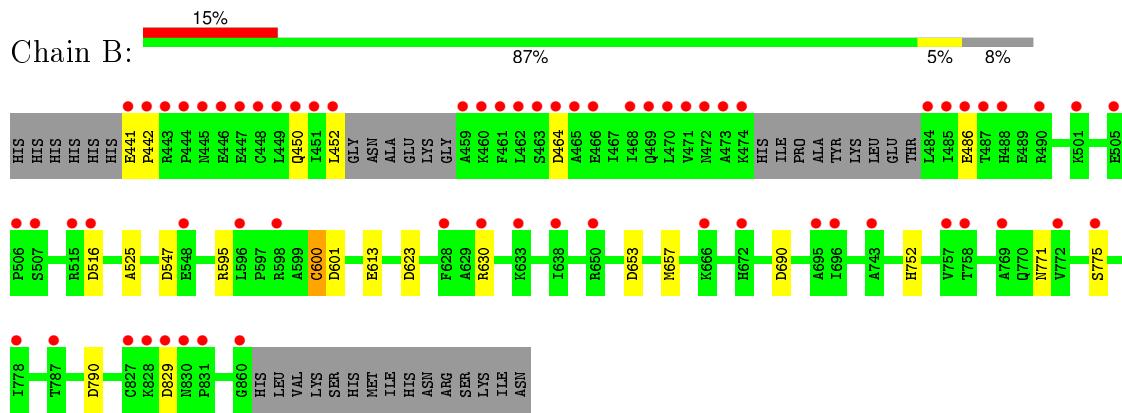
3 Residue-property plots ⓘ

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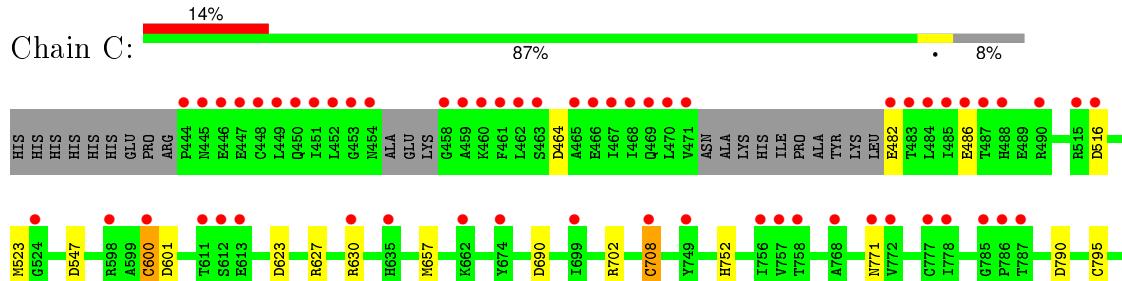
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase
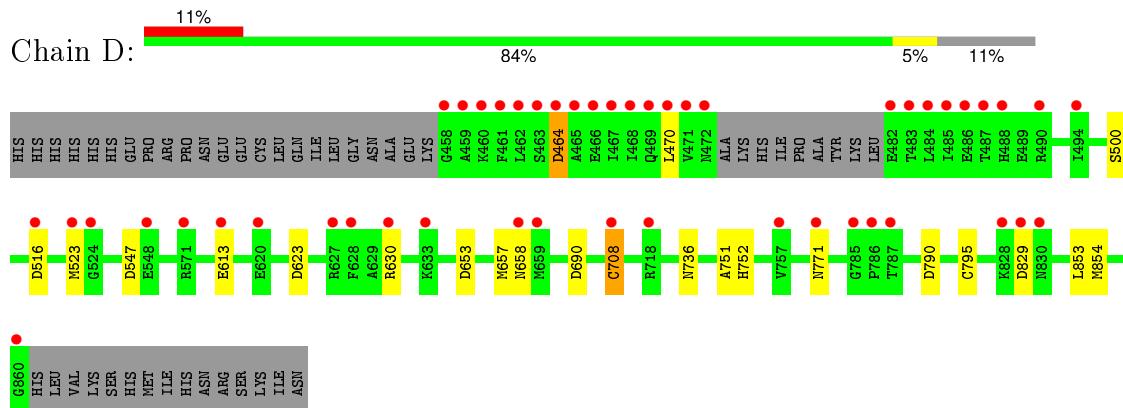
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

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

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

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 0.237 , (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 , 46.3	EDS
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	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.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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

Continued on next page...

Continued from previous page...

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 Too-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 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	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
3	D	38	0	33	0	0
4	A	335	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (49) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 (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	421/441 (96%)	405 (96%)	16 (4%)	0	100	100
1	B	402/441 (91%)	390 (97%)	11 (3%)	1 (0%)	52	32
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%)	56	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	525	ALA

5.3.2 Protein sidechains (i)

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%)	57	36
1	B	326/355 (92%)	318 (98%)	8 (2%)	55	34
1	C	324/355 (91%)	315 (97%)	9 (3%)	51	29
1	D	316/355 (89%)	304 (96%)	12 (4%)	40	17
All	All	1303/1420 (92%)	1266 (97%)	37 (3%)	54	29

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

Continued from previous page...

Mol	Chain	Res	Type
1	C	657	MET
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 (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)

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	0.25	0	6,6,6	0.10	0
3	5HI	A	876	-	33,40,40	0.62	0	40,55,55	1.26	4 (10%)
2	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.08	0
3	5HI	B	876	-	33,40,40	0.63	0	40,55,55	1.42	4 (10%)
2	SO4	C	3	-	4,4,4	0.25	0	6,6,6	0.10	0
3	5HI	C	876	-	33,40,40	0.63	0	40,55,55	1.39	6 (15%)
2	SO4	D	4	-	4,4,4	0.25	0	6,6,6	0.08	0
3	5HI	D	876	-	33,40,40	0.62	1 (3%)	40,55,55	1.46	4 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
3	5HI	A	876	-	-	0/30/35/35	0/3/3/3
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0
3	5HI	B	876	-	-	0/30/35/35	0/3/3/3
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0
3	5HI	C	876	-	-	0/30/35/35	0/3/3/3
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0
3	5HI	D	876	-	-	0/30/35/35	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	876	5HI	C32-C1	-2.06	1.49	1.52

All (18) bond angle outliers are listed below:

Full wwPDB X-ray Structure Validation Report

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	876	5HI	C8-C7-N1	-5.41	107.72	112.29
3	D	876	5HI	C8-C7-N1	-5.29	107.82	112.29
3	C	876	5HI	C8-C7-N1	-5.19	107.91	112.29
3	A	876	5HI	C8-C7-N1	-4.27	108.69	112.29
3	D	876	5HI	C14-C1-N2	-4.12	103.66	109.35
3	C	876	5HI	C14-C1-N2	-3.05	105.13	109.35
3	B	876	5HI	C14-C1-N2	-3.04	105.15	109.35
3	A	876	5HI	C14-C1-N2	-2.57	105.81	109.35
3	B	876	5HI	N3-C5-N1	-2.40	109.12	115.21
3	C	876	5HI	N3-C5-N1	-2.40	109.13	115.21
3	D	876	5HI	N3-C5-N1	-2.39	109.15	115.21
3	A	876	5HI	N3-C5-N1	-2.36	109.23	115.21
3	C	876	5HI	C10-C11-C35	-2.06	109.00	112.94
3	C	876	5HI	C24-C30-C15	-2.04	119.93	122.87
3	B	876	5HI	C24-C30-C15	-2.03	119.95	122.87
3	C	876	5HI	C32-C1-N2	2.10	116.19	111.81
3	D	876	5HI	C32-C1-N2	2.18	116.34	111.81
3	A	876	5HI	C32-C1-N2	2.28	116.55	111.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	876	5HI	1	0
3	C	876	5HI	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	1.11	62 (14%)	3	3	15, 24, 54, 79	0
1	B	405/441 (91%)	1.15	65 (16%)	3	3	14, 24, 80, 99	0
1	C	404/441 (91%)	1.28	62 (15%)	3	3	14, 23, 80, 96	0
1	D	394/441 (89%)	1.08	48 (12%)	5	6	14, 24, 59, 93	0
All	All	1623/1764 (92%)	1.16	237 (14%)	3	4	14, 23, 69, 99	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	461	PHE	12.9
1	B	461	PHE	12.5
1	D	484	LEU	12.0
1	D	461	PHE	11.9
1	D	458	GLY	11.8
1	B	449	LEU	11.7
1	C	453	GLY	11.7
1	A	453	GLY	11.6
1	C	483	THR	11.1
1	C	449	LEU	11.0
1	D	469	GLN	10.7
1	D	470	LEU	10.5
1	C	484	LEU	10.1
1	A	455	ALA	10.0
1	D	462	LEU	9.8
1	C	458	GLY	9.8
1	D	483	THR	9.6
1	D	472	ASN	9.5
1	B	450	GLN	9.2
1	B	474	LYS	9.1
1	C	452	LEU	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	461	PHE	8.4
1	C	462	LEU	8.3
1	C	448	CYS	8.1
1	B	452	LEU	8.0
1	D	468	ILE	8.0
1	C	444	PRO	8.0
1	B	442	PRO	7.7
1	B	451	ILE	7.5
1	C	469	GLN	7.3
1	C	454	ASN	7.1
1	C	487	THR	7.1
1	B	444	PRO	7.1
1	A	442	PRO	7.0
1	C	450	GLN	7.0
1	A	441	GLU	7.0
1	B	448	CYS	6.9
1	C	451	ILE	6.8
1	C	486	GLU	6.8
1	C	446	GLU	6.7
1	B	462	LEU	6.7
1	D	467	ILE	6.7
1	D	459	ALA	6.7
1	D	486	GLU	6.6
1	D	471	VAL	6.6
1	C	471	VAL	6.6
1	C	482	GLU	6.6
1	C	470	LEU	6.5
1	B	441	GLU	6.5
1	A	452	LEU	6.2
1	A	454	ASN	5.9
1	C	445	ASN	5.7
1	D	485	ILE	5.7
1	A	458	GLY	5.7
1	C	447	GLU	5.5
1	A	456	GLU	5.4
1	D	487	THR	5.3
1	A	450	GLN	5.3
1	B	446	GLU	5.1
1	B	484	LEU	5.0
1	C	708[A]	CYS	4.7
1	B	488	HIS	4.6
1	A	635	HIS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	471	VAL	4.5
1	C	488	HIS	4.5
1	B	465	ALA	4.5
1	C	460	LYS	4.4
1	C	786	PRO	4.3
1	D	786	PRO	4.3
1	A	457	LYS	4.3
1	B	828	LYS	4.3
1	B	445	ASN	4.3
1	A	462	LEU	4.2
1	A	786	PRO	4.2
1	A	828	LYS	4.1
1	A	446	GLU	4.1
1	B	447	GLU	4.1
1	B	473	ALA	4.1
1	A	444	PRO	4.0
1	A	785	GLY	4.0
1	B	468	ILE	4.0
1	D	465	ALA	4.0
1	C	829	ASP	4.0
1	C	785	GLY	4.0
1	D	460	LYS	3.9
1	A	787	THR	3.9
1	A	449	LEU	3.8
1	A	484	LEU	3.8
1	A	483	THR	3.8
1	B	485	ILE	3.8
1	B	486	GLU	3.7
1	A	708[A]	CYS	3.7
1	B	470	LEU	3.7
1	C	485	ILE	3.7
1	B	460	LYS	3.7
1	B	829	ASP	3.6
1	A	860	GLY	3.6
1	C	787	THR	3.6
1	C	459	ALA	3.5
1	C	860	GLY	3.5
1	B	516	ASP	3.5
1	C	467	ILE	3.5
1	B	459	ALA	3.4
1	D	466	GLU	3.4
1	B	463	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	828	LYS	3.4
1	C	630	ARG	3.4
1	D	829	ASP	3.4
1	B	772	VAL	3.4
1	A	630	ARG	3.3
1	D	708[A]	CYS	3.3
1	B	506	PRO	3.3
1	B	487	THR	3.3
1	D	627	ARG	3.2
1	D	630	ARG	3.2
1	A	475	HIS	3.1
1	A	718	ARG	3.1
1	B	633	LYS	3.1
1	C	490	ARG	3.0
1	B	743	ALA	3.0
1	D	633	LYS	3.0
1	A	523	MET	3.0
1	A	789	GLU	3.0
1	A	460	LYS	3.0
1	B	466	GLU	3.0
1	A	772	VAL	2.9
1	B	515	ARG	2.9
1	D	463	SER	2.9
1	B	464	ASP	2.9
1	C	463	SER	2.9
1	D	828	LYS	2.9
1	A	829	ASP	2.9
1	C	465	ALA	2.8
1	C	468	ILE	2.8
1	D	482	GLU	2.8
1	D	659	MET	2.8
1	A	633	LYS	2.8
1	B	695	ALA	2.8
1	D	490	ARG	2.8
1	B	831	PRO	2.8
1	A	485	ILE	2.7
1	B	501	LYS	2.7
1	D	613	GLU	2.7
1	A	488	HIS	2.7
1	A	448	CYS	2.7
1	B	827	CYS	2.7
1	A	516	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	620	GLU	2.7
1	B	490	ARG	2.7
1	A	451	ILE	2.7
1	B	469	GLN	2.7
1	C	612	SER	2.7
1	C	768	ALA	2.7
1	C	772	VAL	2.6
1	C	771[A]	ASN	2.6
1	A	515	ARG	2.6
1	D	488	HIS	2.6
1	A	487	THR	2.5
1	A	715	LYS	2.5
1	B	778	ILE	2.5
1	B	830	ASN	2.5
1	B	628	PHE	2.5
1	D	787	THR	2.5
1	A	506	PRO	2.5
1	D	771[A]	ASN	2.5
1	D	860	GLY	2.5
1	C	757	VAL	2.5
1	D	523	MET	2.5
1	A	650	ARG	2.5
1	A	741	ALA	2.5
1	C	466	GLU	2.5
1	C	778	ILE	2.5
1	D	830	ASN	2.4
1	D	516	ASP	2.4
1	C	613	GLU	2.4
1	D	464	ASP	2.4
1	A	695	ALA	2.4
1	C	600[A]	CYS	2.4
1	B	638	ILE	2.4
1	B	472	ASN	2.4
1	B	443	ARG	2.4
1	B	787	THR	2.4
1	D	718	ARG	2.4
1	D	757	VAL	2.4
1	C	516	ASP	2.4
1	D	524	GLY	2.4
1	D	785	GLY	2.4
1	D	658	ASN	2.4
1	A	749	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	749	TYR	2.3
1	A	509	LEU	2.3
1	A	463	SER	2.3
1	D	628	PHE	2.3
1	A	464	ASP	2.3
1	A	468	ILE	2.3
1	D	494	ILE	2.3
1	A	658	ASN	2.3
1	B	505	GLU	2.2
1	A	447	GLU	2.2
1	A	467	ILE	2.2
1	C	699	ILE	2.2
1	A	445	ASN	2.2
1	C	674	TYR	2.2
1	A	768	ALA	2.2
1	C	598	ARG	2.2
1	D	571	ARG	2.2
1	B	696	ILE	2.2
1	C	756	ILE	2.2
1	C	611	THR	2.2
1	B	757	VAL	2.2
1	B	630	ARG	2.2
1	C	662	LYS	2.2
1	C	777	CYS	2.2
1	C	758	THR	2.2
1	A	757	VAL	2.2
1	B	672	HIS	2.2
1	D	548	GLU	2.1
1	B	650	ARG	2.1
1	B	860	GLY	2.1
1	B	758	THR	2.1
1	A	754	ALA	2.1
1	B	666	LYS	2.1
1	A	769	ALA	2.1
1	B	769	ALA	2.1
1	A	486	GLU	2.1
1	B	548	GLU	2.1
1	B	596	LEU	2.1
1	A	627	ARG	2.1
1	C	830	ASN	2.0
1	C	524	GLY	2.0
1	C	635	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	628	PHE	2.0
1	B	507	SER	2.0
1	A	846	VAL	2.0
1	B	598	ARG	2.0
1	C	515	ARG	2.0
1	B	775[A]	SER	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	B	2	5/5	0.70	0.24	5.01	81,81,81,81	0
2	SO4	C	3	5/5	0.76	0.28	4.30	70,70,70,70	0
2	SO4	A	1	5/5	0.66	0.26	3.23	77,77,77,77	0
2	SO4	D	4	5/5	0.75	0.24	2.74	69,69,69,69	0
3	5HI	B	876	38/38	0.86	0.15	1.45	21,29,30,30	0
3	5HI	A	876	38/38	0.87	0.15	0.68	19,25,27,29	0
3	5HI	C	876	38/38	0.86	0.14	0.64	20,27,29,30	0
3	5HI	D	876	38/38	0.86	0.13	0.63	21,27,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.