Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:02 PM GMT

PDB ID	:	1DQ8
Title	:	COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH HMG AND COA
Authors	:	Istvan, E.S.; Palnitkar, M.; Buchanan, S.K.; Deisenhofer, J.
Deposited on	:	1999-12-30
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

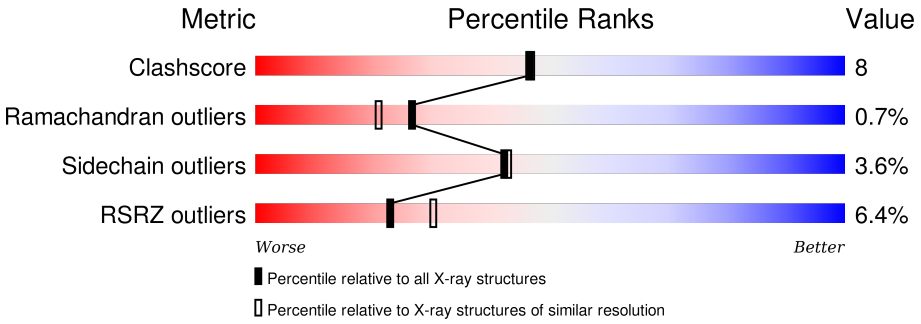
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	467	7% 76% 13% • 11%
1	B	467	6% 72% 12% • 13%
1	C	467	5% 73% 12% • 14%
1	D	467	4% 70% 15% • 13%

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	COA	A	100	X	-	-	-
2	COA	B	101	X	-	-	-
2	COA	C	102	X	-	-	-
2	COA	D	103	X	-	-	-
4	DTT	B	302	-	-	-	X
4	DTT	C	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12667 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.

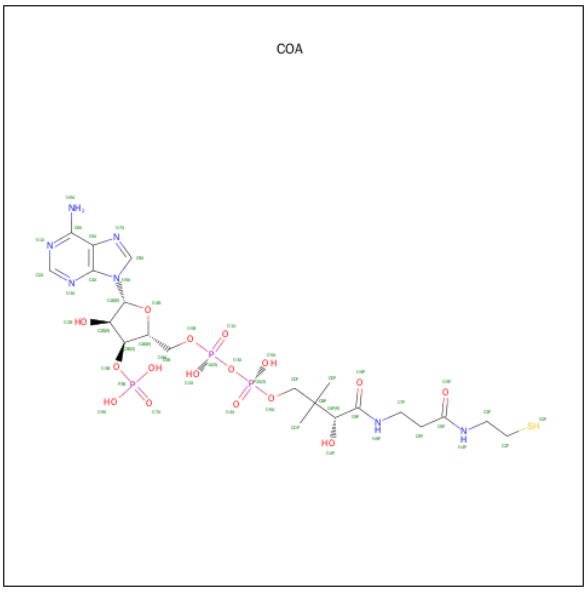
- Molecule 1 is a protein called PROTEIN (HMG-COA REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3114	1942	548	594	30			
1	B	405	Total	C	N	O	S	0	0	0
			3011	1879	528	575	29			
1	C	402	Total	C	N	O	S	0	0	0
			2986	1861	525	571	29			
1	D	407	Total	C	N	O	S	0	0	0
			3023	1887	531	576	29			

There are 4 discrepancies between the modelled and reference sequences:

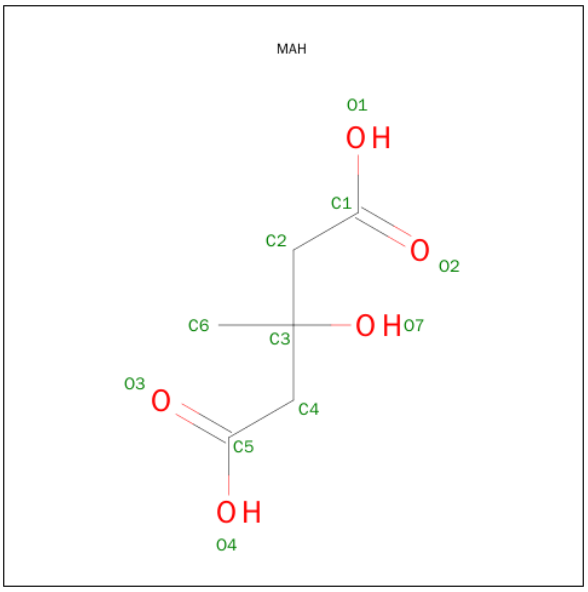
Chain	Residue	Modelled	Actual	Comment	Reference
A	485	ILE	MET	MUTATION	UNP P04035
B	485	ILE	MET	MUTATION	UNP P04035
C	485	ILE	MET	MUTATION	UNP P04035
D	485	ILE	MET	MUTATION	UNP P04035

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



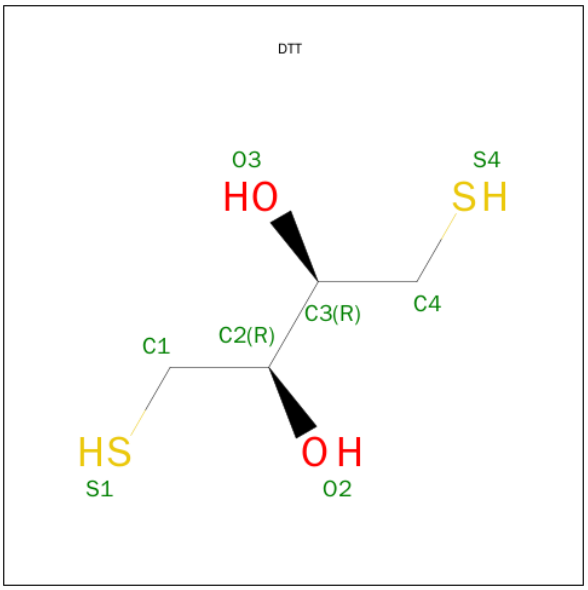
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is 3-HYDROXY-3-METHYL-GLUTARIC ACID (three-letter code: MAH) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O S 8 4 2 2	0	0
4	B	1	Total C O S 8 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	66	Total O 66 66	0	0
5	B	65	Total O 65 65	0	0
5	C	74	Total O 74 74	0	0

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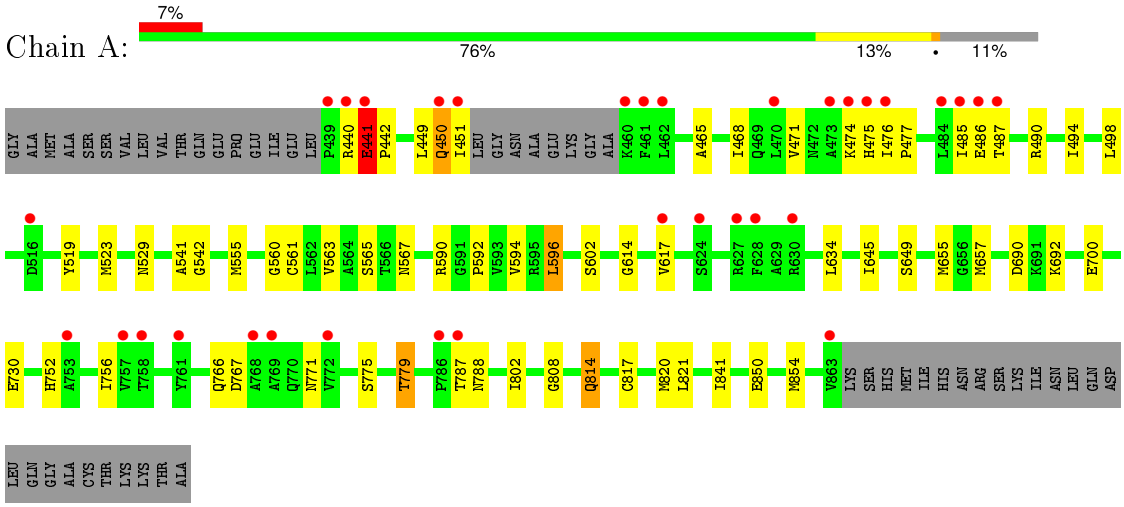
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	76	Total	O	0	0
			76	76		

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.

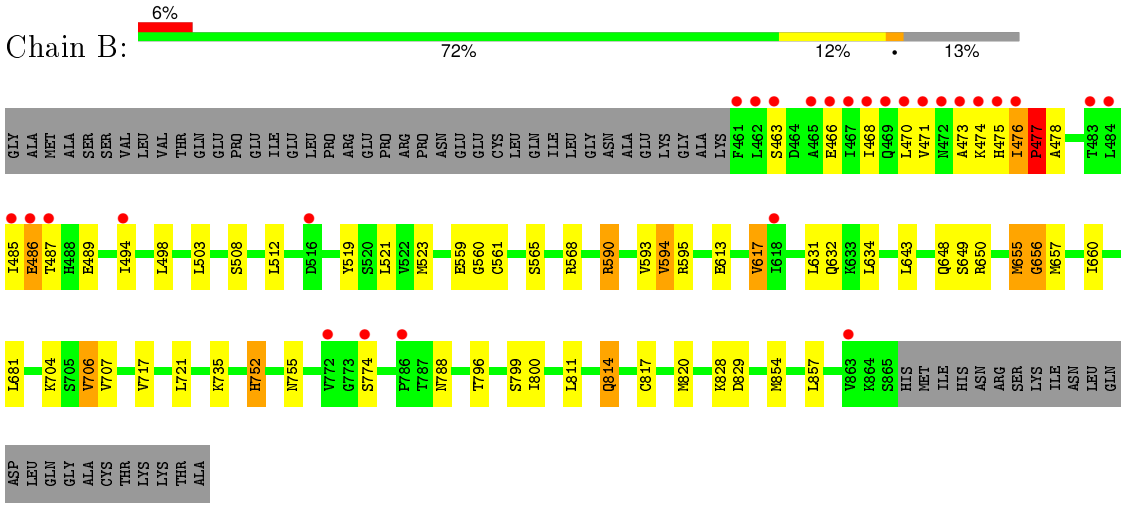
• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

Chain A:



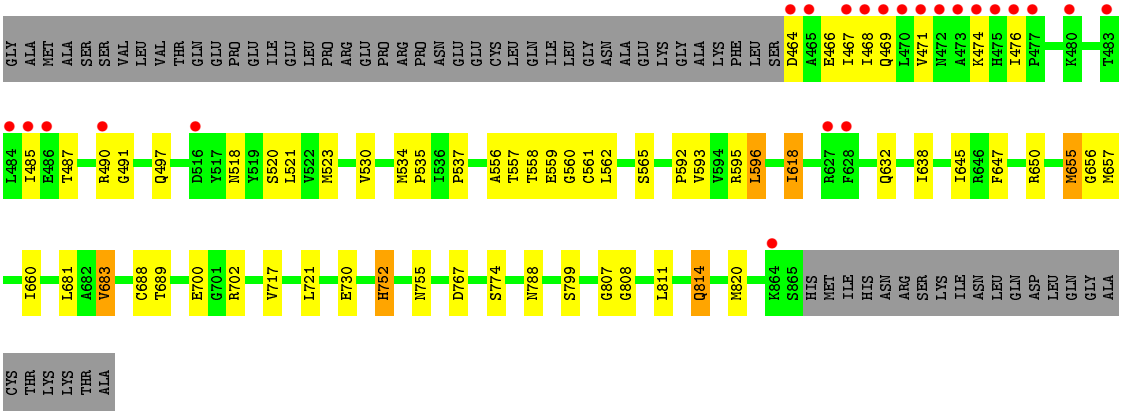
• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

Chain B:



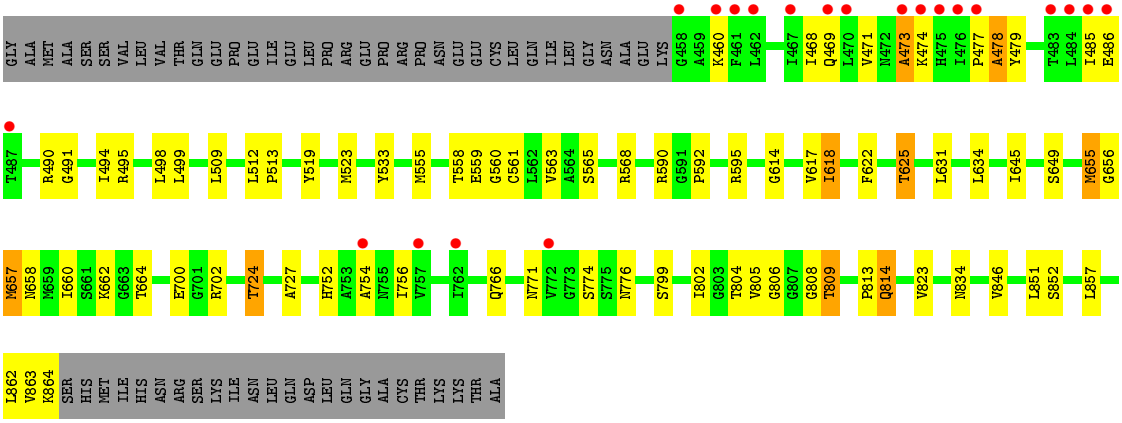
• Molecule 1: PROTEIN (HMG-COA REDUCTASE)

Chain C:



- Molecule 1: PROTEIN (HMG-COA 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	75.30Å 130.18Å 92.55Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	38.00 – 2.10 37.34 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.0 (38.00-2.10) 48.2 (37.34-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.98Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.199 , 0.239 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 56891 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12667	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, MAH, DTT

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	0/3160	0.72	1/4272 (0.0%)
1	B	0.46	0/3055	0.70	1/4131 (0.0%)
1	C	0.48	0/3029	0.69	1/4096 (0.0%)
1	D	0.48	0/3067	0.71	1/4146 (0.0%)
All	All	0.46	0/12311	0.70	4/16645 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	441	GLU	N-CA-C	-7.82	89.90	111.00
1	C	596	LEU	CA-CB-CG	-5.63	102.36	115.30
1	B	656	GLY	N-CA-C	5.45	126.71	113.10
1	D	495	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	3114	0	3155	41	0
1	B	3011	0	3054	47	0
1	C	2986	0	3029	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3023	0	3070	62	0
2	A	48	0	32	1	0
2	B	48	0	32	3	0
2	C	48	0	32	1	0
2	D	48	0	32	3	0
3	A	11	0	8	0	0
3	B	11	0	8	0	0
3	D	22	0	16	0	0
4	B	8	0	10	3	0
4	C	8	0	10	4	0
5	A	66	0	0	1	0
5	B	65	0	0	0	0
5	C	74	0	0	2	0
5	D	76	0	0	3	0
All	All	12667	0	12488	189	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 8.

All (189) 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:C:557:THR:HG22	1:C:559:GLU:H	1.27	0.98
1:C:655:MET:HE1	1:C:657:MET:HB2	1.51	0.92
1:C:534:MET:HE3	1:C:535:PRO:HD2	1.54	0.88
1:C:464:ASP:N	1:C:490:ARG:HH21	1.73	0.86
1:B:854:MET:HE1	1:B:857:LEU:HD12	1.65	0.79
1:D:724:THR:HG22	1:D:727:ALA:H	1.50	0.77
1:A:523:MET:HA	1:A:523:MET:HE3	1.68	0.75
1:C:752:HIS:HD2	1:C:755:ASN:HD22	1.31	0.75
1:A:808:GLY:O	1:A:814:GLN:HG3	1.90	0.72
1:D:485:ILE:HD12	1:D:491:GLY:HA2	1.74	0.70
1:A:779:THR:HG21	1:A:850:GLU:OE1	1.91	0.69
1:D:863:VAL:O	1:D:864:LYS:HB2	1.95	0.66
1:C:632:GLN:HE21	1:C:650:ARG:HG2	1.59	0.66
1:D:806:GLY:O	1:D:809:THR:HB	1.96	0.65
1:C:534:MET:HE3	1:C:535:PRO:CD	2.26	0.65
4:C:301:DTT:S1	1:D:559:GLU:HG3	2.37	0.65
1:C:752:HIS:CD2	1:C:755:ASN:HD22	2.12	0.65
1:C:534:MET:CE	1:D:813:PRO:HB2	2.27	0.64
1:B:655:MET:HE1	1:B:657:MET:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:MET:HE1	1:B:657:MET:HB2	1.79	0.64
1:A:440:ARG:O	1:A:441:GLU:HG2	1.97	0.64
1:B:735:LYS:HE2	1:B:854:MET:HE3	1.78	0.64
1:B:854:MET:CE	1:B:857:LEU:HD12	2.27	0.64
1:C:656:GLY:O	1:C:660:ILE:HG12	1.98	0.64
1:D:477:PRO:HB3	1:D:479:TYR:CE2	2.35	0.62
1:C:534:MET:HE1	1:D:814:GLN:OE1	2.01	0.61
1:A:486:GLU:CD	1:A:486:GLU:H	2.03	0.60
1:C:534:MET:HE1	1:D:813:PRO:HB2	1.83	0.60
1:D:655:MET:HE1	1:D:657:MET:H	1.66	0.60
1:A:468:ILE:HG12	1:A:498:LEU:HD11	1.81	0.60
1:D:592:PRO:HD2	1:D:645:ILE:O	2.01	0.60
1:D:555:MET:HE3	1:D:563:VAL:HA	1.82	0.60
1:D:460:LYS:HB2	1:D:486:GLU:OE1	2.01	0.59
1:B:655:MET:HE1	1:B:657:MET:N	2.17	0.59
1:A:565:SER:HB2	2:A:100:COA:H61	1.85	0.59
1:B:817:CYS:HA	1:B:820:MET:HE3	1.85	0.58
1:A:596:LEU:HD13	1:A:602:SER:HA	1.86	0.58
1:D:519:TYR:O	1:D:523:MET:HG2	2.04	0.57
1:C:534:MET:HE1	1:D:814:GLN:CD	2.25	0.57
1:B:613:GLU:O	1:B:617:VAL:HG13	2.05	0.57
1:B:471:VAL:HG22	1:B:476:ILE:HB	1.87	0.57
1:D:655:MET:HE1	1:D:657:MET:N	2.20	0.56
1:D:555:MET:CE	1:D:563:VAL:HA	2.35	0.56
2:D:103:COA:O4A	2:D:103:COA:H52A	2.06	0.55
1:D:555:MET:HE3	1:D:563:VAL:HG22	1.88	0.55
1:A:542:GLY:H	1:A:567:ASN:ND2	2.04	0.55
1:A:485:ILE:HG21	1:A:490:ARG:HB3	1.87	0.55
1:D:809:THR:HG23	5:D:2076:HOH:O	2.08	0.54
1:C:557:THR:HG21	1:C:562:LEU:HD23	1.89	0.54
1:C:471:VAL:HA	1:C:476:ILE:HG23	1.90	0.54
1:D:499:LEU:HD23	1:D:509:LEU:HD11	1.90	0.54
1:D:485:ILE:HD11	1:D:494:ILE:HD12	1.90	0.53
1:A:475:HIS:O	1:A:477:PRO:HD3	2.07	0.53
1:B:494:ILE:O	1:B:498:LEU:HD13	2.09	0.53
1:D:805:VAL:N	1:D:809:THR:HG21	2.24	0.52
1:C:464:ASP:N	1:C:467:ILE:HG12	2.24	0.52
1:C:485:ILE:HG22	1:C:487:THR:H	1.75	0.52
1:A:592:PRO:HD2	1:A:645:ILE:O	2.10	0.52
1:D:565:SER:HB2	2:D:103:COA:H61	1.92	0.51
1:C:485:ILE:HD12	1:C:491:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:THR:HG21	1:D:823:VAL:HG22	1.91	0.51
1:C:767:ASP:HB2	4:C:301:DTT:H2	1.92	0.51
1:D:631:LEU:HA	1:D:649:SER:HB2	1.93	0.50
1:B:565:SER:HB2	2:B:101:COA:H61	1.93	0.50
1:D:754:ALA:HB1	1:D:771:ASN:HD21	1.77	0.50
1:B:828:LYS:O	1:B:829:ASP:HB2	2.12	0.50
1:A:468:ILE:HG12	1:A:498:LEU:CD1	2.41	0.50
1:B:854:MET:HA	1:B:854:MET:CE	2.42	0.50
1:D:485:ILE:CD1	1:D:494:ILE:HD12	2.41	0.50
1:B:463:SER:OG	1:B:466:GLU:HG3	2.12	0.50
1:C:655:MET:HE1	1:C:657:MET:CB	2.35	0.49
1:B:656:GLY:O	1:B:660:ILE:HG12	2.11	0.49
1:D:808:GLY:O	1:D:814:GLN:HG2	2.13	0.49
1:B:503:LEU:HD13	1:B:508:SER:OG	2.12	0.49
1:A:541:ALA:HB2	1:A:555:MET:HE1	1.94	0.49
1:A:817:CYS:HA	1:A:820:MET:HE3	1.94	0.48
1:A:655:MET:SD	1:A:657:MET:HG2	2.54	0.48
4:C:301:DTT:HO2	1:D:558:THR:HG1	1.61	0.48
1:A:541:ALA:HB2	1:A:555:MET:CE	2.44	0.48
1:D:658:ASN:O	1:D:662:LYS:HG3	2.13	0.48
1:D:804:THR:C	1:D:809:THR:HG21	2.33	0.48
1:D:469:GLN:O	1:D:473:ALA:HB2	2.13	0.48
1:A:771:ASN:OD1	1:A:775:SER:OG	2.32	0.48
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.69	0.48
1:C:466:GLU:HG3	1:C:469:GLN:NE2	2.29	0.48
1:C:565:SER:HB2	2:C:102:COA:H61	1.96	0.47
1:D:655:MET:CE	1:D:657:MET:HG2	2.43	0.47
1:B:468:ILE:HG12	1:B:498:LEU:HD11	1.96	0.47
1:A:821:LEU:HD22	1:A:841:ILE:HD13	1.95	0.47
1:D:592:PRO:HG3	1:D:664:THR:HG21	1.97	0.47
1:D:485:ILE:HG21	1:D:490:ARG:HB3	1.96	0.47
1:D:656:GLY:O	1:D:660:ILE:HG12	2.15	0.47
1:A:614:GLY:O	1:A:617:VAL:HG22	2.15	0.47
1:D:655:MET:HE3	1:D:657:MET:HG2	1.95	0.47
1:A:542:GLY:H	1:A:567:ASN:HD22	1.62	0.47
1:D:823:VAL:O	1:D:823:VAL:HG22	2.15	0.47
1:B:590:ARG:HD3	1:B:590:ARG:HA	1.70	0.47
1:C:592:PRO:HD2	1:C:645:ILE:O	2.15	0.47
1:B:470:LEU:O	1:B:475:HIS:HB2	2.15	0.47
1:A:756:ILE:HD13	5:A:2195:HOH:O	2.15	0.46
1:D:776:ASN:ND2	5:D:2063:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:ARG:HD2	5:D:2044:HOH:O	2.15	0.46
1:B:811:LEU:HB2	1:B:814:GLN:HG2	1.98	0.46
1:C:807:GLY:HA3	4:C:301:DTT:H3	1.97	0.46
1:B:476:ILE:O	1:B:477:PRO:O	2.34	0.46
1:A:767:ASP:OD2	4:B:302:DTT:H11	2.16	0.46
1:C:717:VAL:O	1:C:721:LEU:HB2	2.15	0.46
1:C:820:MET:HE2	1:D:509:LEU:HD21	1.97	0.46
1:B:593:VAL:HG13	1:B:681:LEU:HB3	1.98	0.46
1:B:487:THR:HG22	1:B:489:GLU:N	2.31	0.46
1:D:614:GLY:O	1:D:618:ILE:HG23	2.16	0.46
1:C:774:SER:HA	1:C:799:SER:O	2.16	0.46
1:C:468:ILE:HD11	1:C:497:GLN:HE21	1.80	0.46
1:C:618:ILE:HD13	1:C:647:PHE:HE2	1.80	0.46
1:A:474:LYS:HB2	1:A:476:ILE:CD1	2.46	0.46
1:D:805:VAL:CA	1:D:809:THR:HG21	2.46	0.45
1:D:468:ILE:HG12	1:D:498:LEU:HD12	1.98	0.45
1:D:477:PRO:O	1:D:478:ALA:CB	2.64	0.45
1:A:657:MET:HE2	1:A:690:ASP:CG	2.37	0.45
1:B:752:HIS:HD2	1:B:755:ASN:HD22	1.65	0.45
1:B:468:ILE:HG12	1:B:498:LEU:CD1	2.47	0.45
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.66	0.45
1:A:494:ILE:O	1:A:498:LEU:HD13	2.17	0.45
1:A:555:MET:CE	1:A:563:VAL:HG13	2.46	0.45
1:D:471:VAL:HG11	1:D:498:LEU:HD21	1.98	0.44
1:B:828:LYS:O	1:B:829:ASP:CB	2.66	0.44
1:C:593:VAL:HG13	1:C:681:LEU:HB3	1.98	0.44
1:D:857:LEU:HD21	1:D:862:LEU:HD22	2.00	0.44
1:A:766:GLN:OE1	1:A:802:ILE:HG13	2.17	0.44
1:C:811:LEU:HB2	1:C:814:GLN:HG2	1.99	0.44
1:B:631:LEU:HA	1:B:649:SER:HB2	2.00	0.44
1:A:471:VAL:HG13	1:A:476:ILE:O	2.18	0.44
1:B:476:ILE:N	1:B:477:PRO:HD2	2.33	0.43
1:D:560:GLY:O	1:D:561:CYS:HB2	2.18	0.43
1:B:559:GLU:HB2	4:B:302:DTT:H12	2.00	0.43
1:B:568:ARG:HG3	2:B:101:COA:H4B	2.00	0.43
1:C:534:MET:CE	1:D:814:GLN:NE2	2.81	0.43
1:C:730:GLU:HG2	1:D:595:ARG:HH22	1.83	0.43
1:A:440:ARG:HH22	1:A:465:ALA:H	1.66	0.43
1:C:592:PRO:HG3	1:C:683:VAL:O	2.19	0.43
1:D:468:ILE:HG12	1:D:498:LEU:CD1	2.49	0.43
1:B:632:GLN:HE21	1:B:650:ARG:HE	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:MET:HB2	1:C:820:MET:HE2	1.85	0.42
1:B:485:ILE:HD12	1:B:485:ILE:N	2.34	0.42
1:D:774:SER:HA	1:D:799:SER:O	2.20	0.42
1:D:474:LYS:HE3	1:D:474:LYS:HB2	1.76	0.42
1:C:702:ARG:O	1:C:799:SER:HA	2.20	0.42
1:C:560:GLY:O	1:C:561:CYS:HB2	2.20	0.42
1:A:519:TYR:O	1:A:523:MET:HG2	2.20	0.42
1:C:688:CYS:HB2	1:C:689:THR:CA	2.48	0.42
1:C:523:MET:CE	1:C:530:VAL:HB	2.48	0.42
1:C:656:GLY:HA2	5:C:2097:HOH:O	2.19	0.42
1:B:476:ILE:HG22	1:B:476:ILE:O	2.19	0.42
1:D:568:ARG:HG3	2:D:103:COA:H4B	2.01	0.42
1:A:692:LYS:HB2	1:A:692:LYS:HE2	1.86	0.42
1:B:519:TYR:O	1:B:523:MET:HG2	2.19	0.42
1:C:518:ASN:ND2	1:C:520:SER:OG	2.53	0.42
1:B:473:ALA:O	1:B:475:HIS:N	2.53	0.42
1:A:560:GLY:O	1:A:561:CYS:HB2	2.20	0.42
1:C:537:PRO:O	1:C:556:ALA:HA	2.20	0.41
1:A:767:ASP:HB2	4:B:302:DTT:H2	2.00	0.41
1:B:476:ILE:N	1:B:477:PRO:CD	2.83	0.41
1:D:756:ILE:HG13	1:D:846:VAL:HA	2.02	0.41
1:A:730:GLU:HG2	1:B:595:ARG:HH22	1.85	0.41
1:A:450:GLN:HG3	1:A:451:ILE:H	1.84	0.41
1:B:560:GLY:O	1:B:561:CYS:HB2	2.20	0.41
1:B:594:VAL:HG12	1:B:643:LEU:HB3	2.03	0.41
1:C:464:ASP:N	1:C:490:ARG:NH2	2.55	0.41
1:D:568:ARG:HD3	1:D:852:SER:OG	2.21	0.41
1:A:555:MET:HE3	1:A:563:VAL:HG22	2.03	0.41
1:B:632:GLN:OE1	1:B:648:GLN:HG2	2.20	0.41
1:C:595:ARG:HD2	5:C:2081:HOH:O	2.20	0.41
1:B:706:VAL:HG13	1:B:800:ILE:HD12	2.03	0.41
1:D:823:VAL:CG2	1:D:834:ASN:O	2.69	0.41
1:A:440:ARG:NH2	1:A:465:ALA:H	2.19	0.41
1:D:702:ARG:O	1:D:799:SER:HA	2.21	0.41
1:B:706:VAL:HG23	1:B:707:VAL:N	2.36	0.41
1:D:766:GLN:OE1	1:D:802:ILE:HG13	2.20	0.41
1:B:717:VAL:O	1:B:721:LEU:HB2	2.21	0.41
1:C:557:THR:HG22	1:C:558:THR:N	2.35	0.40
1:C:808:GLY:O	1:C:814:GLN:HG3	2.21	0.40
1:B:655:MET:CE	1:B:657:MET:HB2	2.50	0.40
1:B:568:ARG:HG3	2:B:101:COA:C4B	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:SER:HA	1:B:799:SER:O	2.21	0.40
1:B:796:THR:HG21	1:C:638:ILE:O	2.21	0.40
1:A:850:GLU:O	1:A:854:MET:HG2	2.22	0.40
1:D:622:PHE:O	1:D:625:THR:HB	2.21	0.40
1:A:485:ILE:HG22	1:A:487:THR:H	1.87	0.40
1:D:513:PRO:HB2	1:D:533:TYR:CZ	2.56	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	413/467 (88%)	388 (94%)	21 (5%)	4 (1%)	19	13
1	B	403/467 (86%)	380 (94%)	18 (4%)	5 (1%)	16	10
1	C	400/467 (86%)	383 (96%)	16 (4%)	1 (0%)	46	45
1	D	405/467 (87%)	383 (95%)	20 (5%)	2 (0%)	34	30
All	All	1621/1868 (87%)	1534 (95%)	75 (5%)	12 (1%)	26	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	B	474	LYS
1	B	477	PRO
1	A	441	GLU
1	B	478	ALA
1	D	478	ALA
1	A	449	LEU
1	C	474	LYS
1	A	442	PRO

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Mol	Chain	Res	Type
1	B	486	GLU
1	D	473	ALA
1	B	476	ILE

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	335/375 (89%)	324 (97%)	11 (3%)	45	47
1	B	323/375 (86%)	309 (96%)	14 (4%)	35	34
1	C	320/375 (85%)	311 (97%)	9 (3%)	51	55
1	D	323/375 (86%)	310 (96%)	13 (4%)	38	38
All	All	1301/1500 (87%)	1254 (96%)	47 (4%)	42	43

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	529	ASN
1	A	594	VAL
1	A	596	LEU
1	A	634	LEU
1	A	649	SER
1	A	700	GLU
1	A	752	HIS
1	A	779	THR
1	A	787	THR
1	A	788	ASN
1	A	814	GLN
1	B	477	PRO
1	B	486	GLU
1	B	512	LEU
1	B	521	LEU
1	B	590	ARG
1	B	594	VAL
1	B	617	VAL

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Mol	Chain	Res	Type
1	B	634	LEU
1	B	655	MET
1	B	704	LYS
1	B	706	VAL
1	B	752	HIS
1	B	788	ASN
1	B	814	GLN
1	C	521	LEU
1	C	596	LEU
1	C	618	ILE
1	C	655	MET
1	C	683	VAL
1	C	700	GLU
1	C	752	HIS
1	C	788	ASN
1	C	814	GLN
1	D	512	LEU
1	D	617	VAL
1	D	618	ILE
1	D	625	THR
1	D	634	LEU
1	D	655	MET
1	D	657	MET
1	D	700	GLU
1	D	724	THR
1	D	752	HIS
1	D	809	THR
1	D	814	GLN
1	D	851	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS
1	A	567	ASN
1	A	632	GLN
1	A	788	ASN
1	B	488	HIS
1	B	635	HIS
1	B	752	HIS
1	C	469	GLN
1	C	488	HIS

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Mol	Chain	Res	Type
1	C	497	GLN
1	C	518	ASN
1	C	632	GLN
1	C	752	HIS
1	C	788	ASN
1	D	776	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	COA	A	100	-	40,50,50	1.66	6 (15%)	50,75,75	1.12	6 (12%)
3	MAH	A	200	-	4,10,10	1.62	1 (25%)	2,14,14	0.64	0
2	COA	B	101	-	40,50,50	1.75	5 (12%)	50,75,75	1.47	7 (14%)
3	MAH	B	201	-	4,10,10	1.54	1 (25%)	2,14,14	0.43	0
4	DTT	B	302	-	7,7,7	1.33	0	4,8,8	0.69	0
2	COA	C	102	-	40,50,50	1.67	5 (12%)	50,75,75	1.22	5 (10%)
4	DTT	C	301	-	7,7,7	1.08	0	4,8,8	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	COA	D	103	-	40,50,50	1.78	6 (15%)	50,75,75	1.18	6 (12%)
3	MAH	D	202	-	4,10,10	1.51	1 (25%)	2,14,14	0.51	0
3	MAH	D	203	-	4,10,10	1.77	1 (25%)	2,14,14	0.62	0

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	COA	A	100	-	1/1/11/13	0/44/64/64	0/3/3/3
3	MAH	A	200	-	-	0/6/10/10	0/0/0/0
2	COA	B	101	-	1/1/11/13	0/44/64/64	0/3/3/3
3	MAH	B	201	-	-	0/6/10/10	0/0/0/0
4	DTT	B	302	-	-	0/8/8/8	0/0/0/0
2	COA	C	102	-	1/1/11/13	0/44/64/64	0/3/3/3
4	DTT	C	301	-	-	0/8/8/8	0/0/0/0
2	COA	D	103	-	1/1/11/13	0/44/64/64	0/3/3/3
3	MAH	D	202	-	-	0/6/10/10	0/0/0/0
3	MAH	D	203	-	-	0/6/10/10	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	100	COA	P3B-O8A	2.02	1.62	1.54
2	D	103	COA	P3B-O9A	2.03	1.62	1.54
3	B	201	MAH	C6-C3	2.52	1.55	1.52
2	B	101	COA	P1A-O1A	2.54	1.60	1.51
2	C	102	COA	P2A-O4A	2.58	1.60	1.51
2	A	100	COA	P1A-O1A	2.60	1.60	1.51
2	C	102	COA	C5A-C4A	2.65	1.46	1.40
2	C	102	COA	P1A-O1A	2.66	1.60	1.51
2	A	100	COA	P2A-O4A	2.67	1.60	1.51
2	C	102	COA	P3B-O7A	2.68	1.60	1.51
2	B	101	COA	C5A-C4A	2.69	1.46	1.40
2	B	101	COA	P2A-O4A	2.70	1.61	1.51
2	D	103	COA	P2A-O4A	2.71	1.61	1.51
2	A	100	COA	C5A-C4A	2.72	1.46	1.40
2	D	103	COA	P1A-O1A	2.79	1.61	1.51
2	D	103	COA	C5A-C4A	2.81	1.46	1.40
3	D	202	MAH	C6-C3	2.83	1.55	1.52
2	D	103	COA	P3B-O7A	2.95	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	COA	P3B-O7A	3.01	1.61	1.51
3	A	200	MAH	C6-C3	3.05	1.55	1.52
3	D	203	MAH	C6-C3	3.10	1.55	1.52
2	A	100	COA	P3B-O7A	3.19	1.61	1.51
2	A	100	COA	C4A-N3A	7.07	1.46	1.35
2	C	102	COA	C4A-N3A	7.43	1.46	1.35
2	D	103	COA	C4A-N3A	7.59	1.46	1.35
2	B	101	COA	C4A-N3A	7.78	1.47	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	100	COA	P2A-O3A-P1A	-2.69	125.17	132.73
2	A	100	COA	O5P-C5P-C6P	-2.34	117.94	121.98
2	B	101	COA	O5P-C5P-C6P	-2.23	118.13	121.98
2	D	103	COA	O5P-C5P-C6P	-2.22	118.16	121.98
2	C	102	COA	O5P-C5P-C6P	-2.13	118.31	121.98
2	D	103	COA	P2A-O3A-P1A	-2.09	126.87	132.73
2	A	100	COA	C7P-N8P-C9P	-2.08	118.41	122.53
2	A	100	COA	C3B-C2B-C1B	2.05	104.89	99.98
2	C	102	COA	C3B-C2B-C1B	2.19	105.24	99.98
2	A	100	COA	C4A-C5A-N7A	2.22	111.52	109.48
2	D	103	COA	C3B-C2B-C1B	2.28	105.45	99.98
2	D	103	COA	C4A-C5A-N7A	2.32	111.62	109.48
2	B	101	COA	C3B-C2B-C1B	2.44	105.84	99.98
2	D	103	COA	C4B-O4B-C1B	2.49	112.45	109.72
2	B	101	COA	O6A-CCP-CBP	2.59	114.70	110.55
2	A	100	COA	O3A-P1A-O5B	2.60	109.83	102.94
2	B	101	COA	C4B-O4B-C1B	2.66	112.64	109.72
2	C	102	COA	C4B-O4B-C1B	2.74	112.73	109.72
2	C	102	COA	C4A-C5A-N7A	2.78	112.03	109.48
2	B	101	COA	C4A-C5A-N7A	3.12	112.35	109.48
2	D	103	COA	O3A-P1A-O5B	3.85	113.15	102.94
2	C	102	COA	O3A-P1A-O5B	3.94	113.40	102.94
2	B	101	COA	O3A-P2A-O6A	4.12	113.87	102.94
2	B	101	COA	O3A-P1A-O5B	4.78	115.62	102.94

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	100	COA	C3B
2	D	103	COA	C3B

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Mol	Chain	Res	Type	Atom
2	C	102	COA	C3B
2	B	101	COA	C3B

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	100	COA	1	0
2	B	101	COA	3	0
4	B	302	DTT	3	0
2	C	102	COA	1	0
4	C	301	DTT	4	0
2	D	103	COA	3	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, 95^{th} 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	417/467 (89%)	0.24	33 (7%)	15	21	19, 34, 62, 79	0
1	B	405/467 (86%)	0.21	27 (6%)	21	28	19, 32, 66, 80	0
1	C	402/467 (86%)	0.10	23 (5%)	27	35	17, 29, 69, 93	0
1	D	407/467 (87%)	-0.01	21 (5%)	31	39	19, 30, 59, 76	0
All	All	1631/1868 (87%)	0.13	104 (6%)	23	30	17, 32, 64, 93	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	ILE	9.3
1	B	461	PHE	8.5
1	C	470	LEU	8.1
1	C	485	ILE	7.8
1	C	475	HIS	7.0
1	B	484	LEU	6.9
1	C	473	ALA	6.7
1	C	484	LEU	6.7
1	D	473	ALA	6.5
1	B	473	ALA	6.3
1	C	464	ASP	6.3
1	C	476	ILE	6.1
1	B	476	ILE	6.0
1	B	485	ILE	6.0
1	A	461	PHE	5.9
1	C	471	VAL	5.8
1	C	483	THR	5.6
1	D	470	LEU	5.6
1	B	470	LEU	5.4
1	B	487	THR	5.1
1	A	439	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	471	VAL	5.0
1	C	486	GLU	4.9
1	C	467	ILE	4.7
1	A	462	LEU	4.7
1	C	627	ARG	4.7
1	B	863	VAL	4.7
1	D	461	PHE	4.6
1	C	472	ASN	4.4
1	C	469	GLN	4.4
1	B	472	ASN	4.2
1	A	450	GLN	4.1
1	B	462	LEU	4.1
1	A	627	ARG	4.0
1	D	484	LEU	4.0
1	A	440	ARG	3.9
1	A	460	LYS	3.9
1	B	786	PRO	3.8
1	C	465	ALA	3.8
1	A	484	LEU	3.8
1	D	462	LEU	3.7
1	B	483	THR	3.6
1	B	516	ASP	3.6
1	B	468	ILE	3.6
1	B	475	HIS	3.5
1	B	469	GLN	3.5
1	A	476	ILE	3.4
1	D	486	GLU	3.4
1	B	474	LYS	3.3
1	D	483	THR	3.3
1	D	474	LYS	3.3
1	A	772	VAL	3.3
1	D	772	VAL	3.3
1	B	465	ALA	3.3
1	B	466	GLU	3.2
1	B	772	VAL	3.2
1	D	476	ILE	3.2
1	A	475	HIS	3.1
1	D	469	GLN	3.1
1	A	486	GLU	3.0
1	B	467	ILE	3.0
1	C	480	LYS	3.0
1	D	485	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	487	THR	3.0
1	C	468	ILE	2.9
1	B	486	GLU	2.9
1	C	477	PRO	2.8
1	A	787	THR	2.8
1	A	768	ALA	2.7
1	A	485	ILE	2.7
1	A	786	PRO	2.7
1	C	628	PHE	2.6
1	B	494	ILE	2.6
1	A	473	ALA	2.6
1	A	487	THR	2.6
1	C	864	LYS	2.5
1	A	624	SER	2.5
1	D	477	PRO	2.5
1	A	516	ASP	2.4
1	D	475	HIS	2.4
1	A	761	TYR	2.4
1	A	757	VAL	2.4
1	A	863	VAL	2.4
1	A	753	ALA	2.4
1	B	618	ILE	2.4
1	A	628	PHE	2.3
1	A	769	ALA	2.3
1	D	762	ILE	2.3
1	C	490	ARG	2.3
1	C	516	ASP	2.3
1	D	754	ALA	2.3
1	D	757	VAL	2.2
1	A	470	LEU	2.2
1	A	630	ARG	2.2
1	C	474	LYS	2.2
1	D	458	GLY	2.1
1	A	617	VAL	2.1
1	A	441	GLU	2.1
1	B	463	SER	2.1
1	A	758	THR	2.1
1	D	460	LYS	2.1
1	A	474	LYS	2.1
1	B	774	SER	2.0
1	D	467	ILE	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, 95^{th} 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
4	DTT	B	302	8/8	0.83	0.19	2.20	70,72,74,79	0
4	DTT	C	301	8/8	0.90	0.15	1.40	68,70,72,75	0
3	MAH	B	201	11/11	0.97	0.13	0.08	31,34,35,36	0
2	COA	C	102	48/48	0.96	0.09	-0.20	27,33,44,48	0
3	MAH	D	202	11/11	0.96	0.11	-0.38	23,30,33,35	0
2	COA	B	101	48/48	0.95	0.09	-0.47	37,44,54,55	0
3	MAH	D	203	11/11	0.98	0.11	-0.47	32,36,37,37	0
2	COA	D	103	48/48	0.95	0.09	-0.51	35,42,51,52	0
3	MAH	A	200	11/11	0.95	0.12	-0.52	31,39,41,42	0
2	COA	A	100	48/48	0.95	0.09	-0.80	35,40,51,53	0

6.5 Other polymers (i)

There are no such residues in this entry.