Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:57 PM GMT

PDB ID	:	4UBT
Title	:	Structure of the C93S variant of the 3-ketoacyl-CoA thiolase FadA5 from M. tuberculosis in complex with a steroid and CoA.
Authors	:	Schaefer, C.M.; Kisker, C.
Deposited on	:	2014-08-13
Resolution	:	1.70 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:

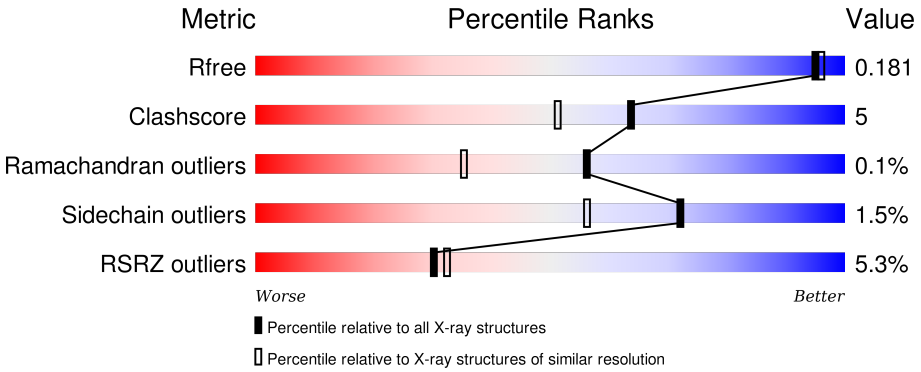
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3190 (1.70-1.70)
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	399	7%, 89%, 10%
1	B	399	5%, 89%, 8%
1	C	399	5%, 89%, 9%
1	D	399	5%, 86%, 8%, 6%

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	D	401[A]	-	-	-	X
2	COA	D	401[B]	-	-	-	X
3	3G6	B	402	-	-	-	X
4	GOL	A	403	-	-	-	X
4	GOL	A	405[A]	-	-	-	X
4	GOL	A	405[B]	-	-	-	X
4	GOL	C	403[A]	-	-	-	X
4	GOL	C	403[B]	-	-	-	X
4	GOL	D	402[A]	-	-	-	X
4	GOL	D	402[B]	-	-	-	X
5	CL	D	403	-	-	-	X
6	PEG	C	404	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13460 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 Acetyl-CoA acetyltransferase FadA5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	20	0
			3065	1898	572	583	12			
1	B	392	Total	C	N	O	S	0	14	0
			2993	1851	555	574	13			
1	C	391	Total	C	N	O	S	0	18	0
			3001	1860	551	578	12			
1	D	376	Total	C	N	O	S	0	19	0
			2894	1801	527	554	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP I6XHI4
A	-6	HIS	-	expression tag	UNP I6XHI4
A	-5	HIS	-	expression tag	UNP I6XHI4
A	-4	HIS	-	expression tag	UNP I6XHI4
A	-3	HIS	-	expression tag	UNP I6XHI4
A	-2	HIS	-	expression tag	UNP I6XHI4
A	-1	GLY	-	expression tag	UNP I6XHI4
A	0	SER	-	expression tag	UNP I6XHI4
A	93	SER	CYS	engineered mutation	UNP I6XHI4
B	-7	HIS	-	expression tag	UNP I6XHI4
B	-6	HIS	-	expression tag	UNP I6XHI4
B	-5	HIS	-	expression tag	UNP I6XHI4
B	-4	HIS	-	expression tag	UNP I6XHI4
B	-3	HIS	-	expression tag	UNP I6XHI4
B	-2	HIS	-	expression tag	UNP I6XHI4
B	-1	GLY	-	expression tag	UNP I6XHI4
B	0	SER	-	expression tag	UNP I6XHI4
B	93	SER	CYS	engineered mutation	UNP I6XHI4
C	-7	HIS	-	expression tag	UNP I6XHI4
C	-6	HIS	-	expression tag	UNP I6XHI4
C	-5	HIS	-	expression tag	UNP I6XHI4

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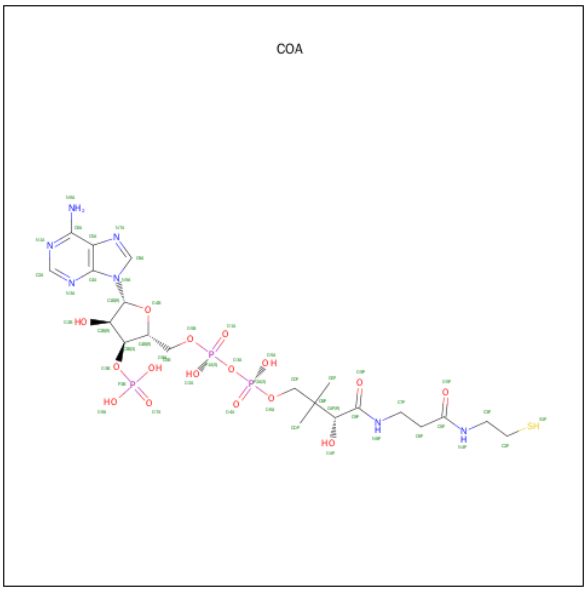
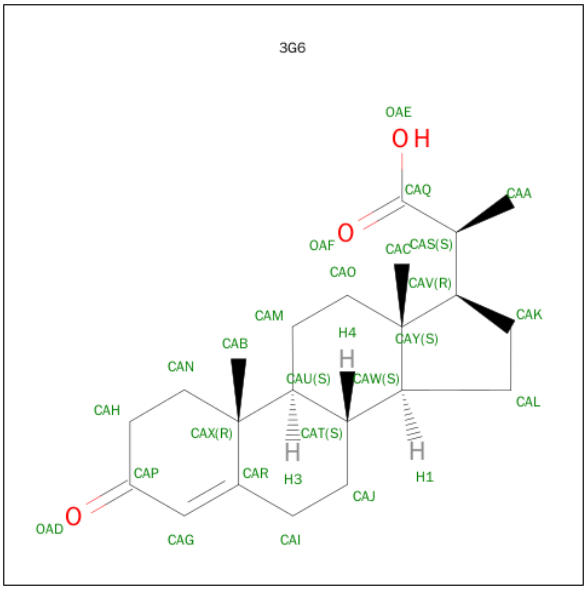
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP I6XHI4
C	-3	HIS	-	expression tag	UNP I6XHI4
C	-2	HIS	-	expression tag	UNP I6XHI4
C	-1	GLY	-	expression tag	UNP I6XHI4
C	0	SER	-	expression tag	UNP I6XHI4
C	93	SER	CYS	engineered mutation	UNP I6XHI4
D	-7	HIS	-	expression tag	UNP I6XHI4
D	-6	HIS	-	expression tag	UNP I6XHI4
D	-5	HIS	-	expression tag	UNP I6XHI4
D	-4	HIS	-	expression tag	UNP I6XHI4
D	-3	HIS	-	expression tag	UNP I6XHI4
D	-2	HIS	-	expression tag	UNP I6XHI4
D	-1	GLY	-	expression tag	UNP I6XHI4
D	0	SER	-	expression tag	UNP I6XHI4
D	93	SER	CYS	engineered mutation	UNP I6XHI4

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



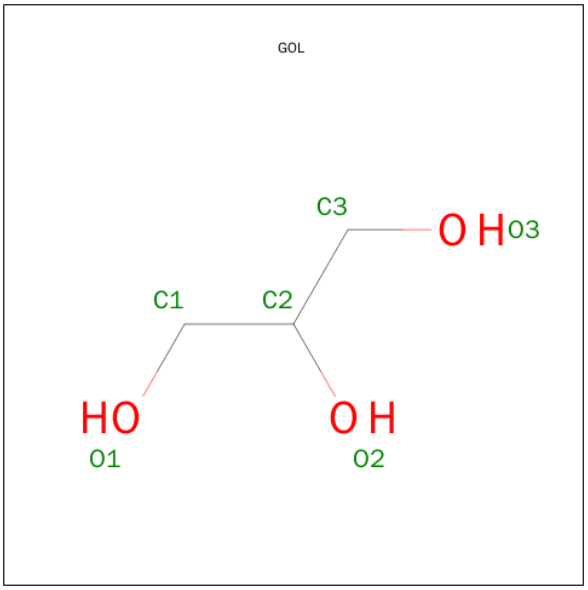
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	1
			52	23	8	16	3	2		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	1
			57	26	9	17	3	2		

- Molecule 3 is (2S)-2-[(8S,9S,10R,13S,14S,17R)-10,13-dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]propanoic acid (non-preferred name) (three-letter code: 3G6) (formula: $C_{22}H_{32}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 22 3	0	0
3	B	1	Total C O 25 22 3	0	0
3	C	1	Total C O 25 22 3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

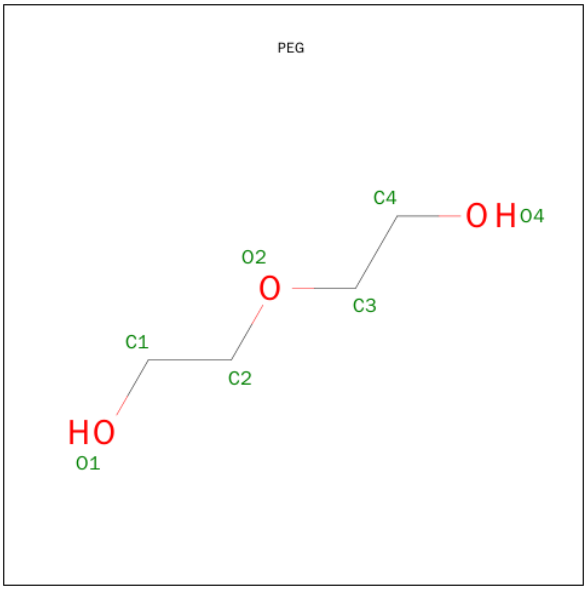


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 12 6 6	0	1
4	C	1	Total C O 12 6 6	0	1
4	D	1	Total C O 12 6 6	0	1

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	5	Total Cl 5 5	0	0
5	A	2	Total Cl 2 2	0	0
5	D	2	Total Cl 2 2	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Na 1 1	0	0

- Molecule 8 is water.

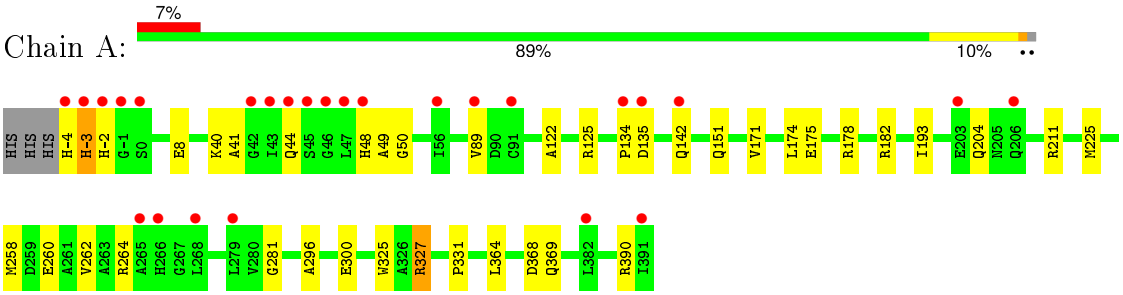
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	304	Total O 304 304	0	0
8	B	312	Total O 312 312	0	0
8	C	282	Total O 282 282	0	0
8	D	263	Total O 263 263	0	0

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.

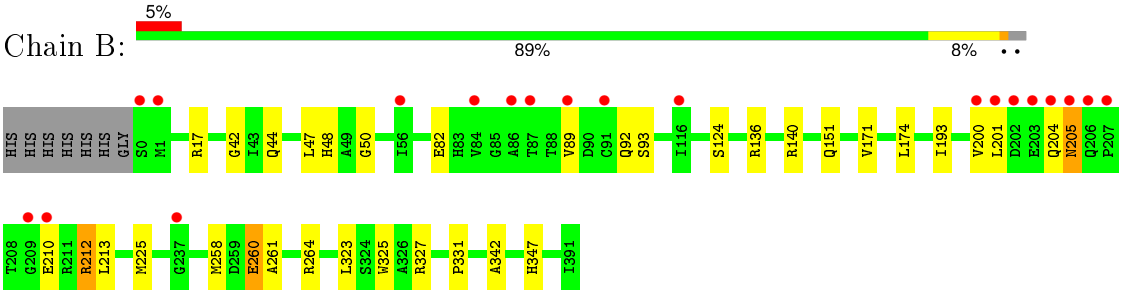
- Molecule 1: Acetyl-CoA acetyltransferase FadA5

Chain A:



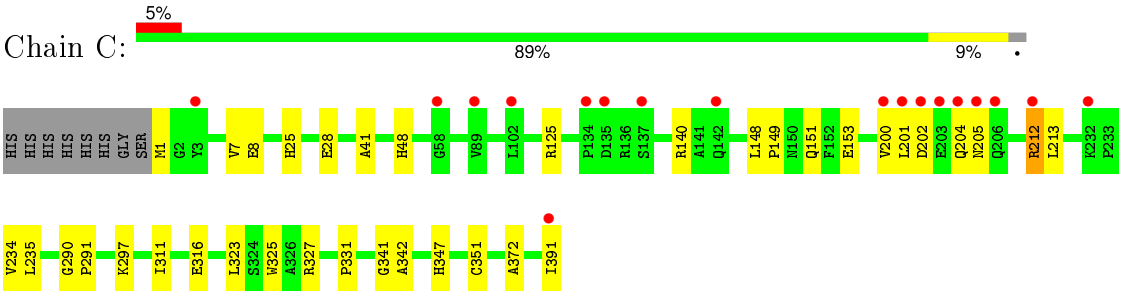
- Molecule 1: Acetyl-CoA acetyltransferase FadA5

Chain B:



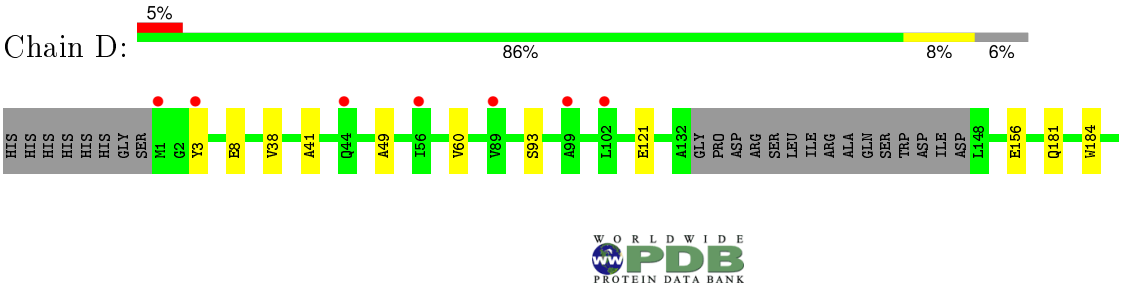
- Molecule 1: Acetyl-CoA acetyltransferase FadA5

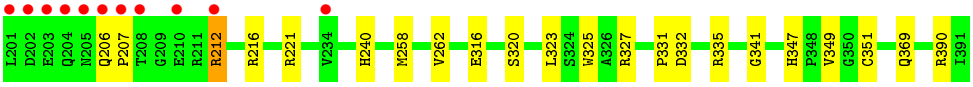
Chain C:



- Molecule 1: Acetyl-CoA acetyltransferase FadA5

Chain D:




L201
D202
E203
Q204
N205
Q206
P207
T208
G209
E210
R211
R212
R216
R221
Y234
H240
M258
V262
E316
S320
L323
S324
W325
A326
R327
P331
D332
R335
G341
H347
P348
V349
G350
C351
Q369
R390
I391

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.66Å 100.18Å 107.95Å 90.00° 99.90° 90.00°	Depositor
Resolution (Å)	37.68 – 1.70 47.49 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.68-1.70) 99.7 (47.49-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.145 , 0.174 0.153 , 0.181	Depositor DCC
R_{free} test set	8796 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 175700 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13460	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: GOL, CL, NA, 3G6, COA, PEG

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	0.35	0/3159	0.52	0/4279
1	B	0.34	0/3065	0.52	0/4152
1	C	0.33	0/3080	0.52	0/4176
1	D	0.35	0/2984	0.53	0/4039
All	All	0.34	0/12288	0.52	0/16646

There are no bond length outliers.

There are no bond angle outliers.

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	3065	0	3084	33	2
1	B	2993	0	3000	34	0
1	C	3001	0	3006	36	0
1	D	2894	0	2942	25	0
2	A	48	0	32	0	0
2	B	52	0	12	0	0
2	C	48	0	32	0	0
2	D	57	0	22	0	0
3	A	25	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	31	5	0
3	C	25	0	31	1	0
4	A	24	0	32	0	0
4	C	12	0	16	0	0
4	D	12	0	16	1	2
5	A	2	0	0	1	0
5	B	5	0	0	2	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	C	7	0	10	1	0
7	C	1	0	0	0	0
8	A	304	0	0	7	0
8	B	312	0	0	6	0
8	C	282	0	0	5	1
8	D	263	0	0	0	1
All	All	13460	0	12297	129	3

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 5.

All (129) 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:204:GLN:N	1:A:204:GLN:OE1	1.96	0.98
1:C:234[B]:VAL:O	8:C:776:HOH:O	1.83	0.97
1:A:134[A]:PRO:O	8:A:783:HOH:O	1.87	0.93
1:B:17[D]:ARG:HH21	1:B:17[D]:ARG:HG2	1.34	0.91
1:A:327[A]:ARG:CG	1:A:327[A]:ARG:HH21	1.86	0.88
1:B:204:GLN:O	1:B:205:ASN:HB2	1.74	0.86
1:B:17[D]:ARG:CG	1:B:17[D]:ARG:HH21	1.91	0.83
1:C:200:VAL:CG2	1:C:212[A]:ARG:HG3	2.10	0.81
1:A:48[A]:HIS:CD2	1:A:50:GLY:H	2.01	0.78
1:B:323:LEU:O	1:B:327:ARG:HG2	1.85	0.76
1:A:182:ARG:NH1	8:A:788:HOH:O	2.20	0.74
1:D:212[A]:ARG:CG	1:D:212[A]:ARG:HH11	2.02	0.73
1:C:323:LEU:O	1:C:327:ARG:HG3	1.90	0.72
1:A:48[A]:HIS:ND1	5:A:407:CL:CL	2.60	0.71
1:A:327[A]:ARG:HG2	1:A:327[A]:ARG:HH21	1.55	0.69
1:C:200:VAL:HG22	1:C:212[A]:ARG:CG	2.24	0.68
1:A:369:GLN:O	1:A:390:ARG:HD3	1.94	0.67
1:B:44:GLN:OE1	8:B:722:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327[A]:ARG:CG	1:A:327[A]:ARG:NH2	2.52	0.67
1:C:200:VAL:CG2	1:C:212[A]:ARG:CG	2.74	0.66
1:C:200:VAL:HG22	1:C:212[A]:ARG:HG3	1.77	0.65
1:C:200:VAL:HG23	1:C:212[A]:ARG:HG3	1.77	0.64
1:A:327[A]:ARG:HG3	1:A:327[A]:ARG:NH2	2.12	0.63
1:A:300[B]:GLU:HG3	8:A:768:HOH:O	1.98	0.63
1:C:234[B]:VAL:O	1:C:235[B]:LEU:HB2	1.97	0.63
1:B:204:GLN:O	1:B:205:ASN:CB	2.46	0.62
1:C:140:ARG:NH2	8:C:501:HOH:O	2.32	0.62
1:A:135[B]:ASP:N	8:A:783:HOH:O	2.26	0.62
1:C:25[B]:HIS:CE1	1:C:125:ARG:NH2	2.67	0.62
1:B:48[B]:HIS:NE2	5:B:404:CL:CL	2.55	0.62
1:D:156:GLU:HB3	4:D:402[B]:GOL:H31	1.83	0.60
1:B:200:VAL:HB	1:B:210:GLU:HB2	1.82	0.60
1:A:89:VAL:HG12	1:B:89:VAL:HG12	1.82	0.60
1:D:323:LEU:O	1:D:327:ARG:HG3	2.01	0.60
1:A:-4:HIS:O	1:A:-3:HIS:HB3	2.01	0.60
1:C:391[A]:ILE:HG22	1:C:391[A]:ILE:O	2.00	0.60
1:C:202[B]:ASP:OD1	1:C:205:ASN:N	2.35	0.60
1:A:-4:HIS:O	1:A:-3:HIS:CB	2.49	0.60
1:C:7:VAL:O	1:C:8[A]:GLU:HG2	2.03	0.59
1:A:327[A]:ARG:HG3	1:A:327[A]:ARG:HH21	1.64	0.57
1:D:212[A]:ARG:CG	1:D:212[A]:ARG:NH1	2.65	0.57
1:D:60:VAL:HG21	1:D:349[B]:VAL:HG12	1.87	0.57
1:A:8[A]:GLU:HG3	1:A:41:ALA:HB2	1.87	0.57
1:B:48[B]:HIS:CD2	1:B:50[B]:GLY:H	2.23	0.56
1:B:140:ARG:NH1	5:B:407:CL:CL	2.73	0.56
1:A:40:LYS:NZ	8:A:691:HOH:O	2.36	0.55
1:A:260:GLU:OE2	1:A:264:ARG:NH2	2.36	0.55
1:D:60:VAL:HG21	1:D:349[B]:VAL:CG1	2.35	0.55
1:D:325:TRP:CZ3	1:D:331:PRO:HG3	2.42	0.55
1:D:8[A]:GLU:HG3	1:D:41:ALA:HB2	1.89	0.54
1:B:17[D]:ARG:NH1	8:B:772:HOH:O	2.40	0.54
1:C:8[A]:GLU:HG3	1:C:41:ALA:HB2	1.89	0.53
1:B:174:LEU:HD22	1:B:225[B]:MET:HG2	1.89	0.53
1:D:212[A]:ARG:HG3	1:D:212[A]:ARG:HH11	1.74	0.53
1:A:44:GLN:OE1	1:A:44:GLN:HA	2.09	0.53
1:D:212[A]:ARG:HG2	1:D:212[A]:ARG:NH1	2.24	0.52
1:B:325:TRP:CZ3	1:B:331:PRO:HG3	2.44	0.52
1:C:140:ARG:HH11	1:C:148:LEU:HD23	1.75	0.52
1:B:201:LEU:HD22	1:B:201:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLN:HB3	3:B:402:3G6:H11	1.91	0.51
1:B:17[D]:ARG:NH2	1:B:17[D]:ARG:CG	2.58	0.51
1:C:200:VAL:HG22	1:C:212[A]:ARG:HG2	1.93	0.51
1:C:149:PRO:HB2	1:C:153[A]:GLU:HB2	1.93	0.51
1:C:25[A]:HIS:HB3	1:C:28:GLU:HG3	1.92	0.50
6:C:404:PEG:H12	8:C:660:HOH:O	2.12	0.50
1:B:342:ALA:HB1	1:B:347:HIS:HB2	1.93	0.50
1:B:92:GLN:HB3	3:B:402:3G6:OAE	2.12	0.50
1:A:296:ALA:O	1:A:300[B]:GLU:HG3	2.12	0.50
1:B:225[B]:MET:HE3	1:B:225[B]:MET:HA	1.94	0.49
3:B:402:3G6:H16	3:B:402:3G6:H7	1.93	0.49
1:C:325:TRP:CZ3	1:C:331:PRO:HG3	2.46	0.49
1:B:212[A]:ARG:NH1	8:B:716:HOH:O	2.45	0.49
1:B:260[A]:GLU:HG3	1:B:261:ALA:N	2.27	0.49
1:B:260[B]:GLU:OE2	1:B:264:ARG:HD2	2.12	0.49
1:A:-4:HIS:O	1:A:-3:HIS:CG	2.67	0.48
1:A:174:LEU:HD22	1:A:225:MET:HG2	1.95	0.48
1:D:3:TYR:N	1:D:3:TYR:CD1	2.81	0.48
1:D:316:GLU:CD	1:D:341:GLY:HA3	2.34	0.48
1:C:140:ARG:NH1	1:C:148:LEU:HD23	2.29	0.48
1:C:151:GLN:HB3	3:C:401:3G6:H11	1.96	0.47
1:C:202[A]:ASP:HB3	1:C:204:GLN:H	1.80	0.47
1:B:124:SER:HB2	8:B:627:HOH:O	2.14	0.47
1:C:25[B]:HIS:CE1	1:C:125:ARG:HH21	2.32	0.47
1:A:122:ALA:HB1	8:A:804:HOH:O	2.15	0.47
1:D:121:GLU:HG2	1:D:349[A]:VAL:HG22	1.97	0.47
1:B:171:VAL:HG22	1:B:225[A]:MET:HE3	1.96	0.47
1:D:38:VAL:HG11	1:D:49:ALA:HB2	1.96	0.46
1:A:151:GLN:HB3	3:A:402:3G6:H11	1.97	0.46
1:A:48[A]:HIS:CG	1:A:49:ALA:N	2.84	0.46
1:D:93[B]:SER:OG	1:D:349[B]:VAL:HG13	2.16	0.46
1:A:325:TRP:CZ3	1:A:331:PRO:HG3	2.50	0.46
1:A:171:VAL:O	1:A:175[B]:GLU:HG3	2.16	0.46
1:C:234[B]:VAL:O	1:C:235[B]:LEU:CB	2.64	0.45
1:B:212[A]:ARG:NH1	1:B:213:LEU:O	2.48	0.45
1:C:48[A]:HIS:CD2	8:C:779:HOH:O	2.70	0.45
1:B:47:LEU:HD13	1:B:258:MET:HE1	1.97	0.45
1:A:258:MET:CE	1:A:262:VAL:HG12	2.46	0.45
1:D:258:MET:CE	1:D:262:VAL:HG12	2.46	0.45
1:B:42:GLY:O	8:B:726:HOH:O	2.21	0.45
1:C:297:LYS:NZ	8:C:503:HOH:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212[A]:ARG:HG2	1:D:212[A]:ARG:HH11	1.79	0.44
1:C:290:GLY:N	1:C:291:PRO:CD	2.80	0.44
1:D:369:GLN:O	1:D:390:ARG:HD3	2.17	0.44
1:C:316:GLU:CD	1:C:341:GLY:HA3	2.39	0.43
1:A:364:LEU:HB3	1:A:390:ARG:HD2	2.00	0.43
1:C:342:ALA:HB1	1:C:347:HIS:HB2	2.00	0.43
1:D:258:MET:HE2	1:D:262:VAL:HG12	2.00	0.43
1:C:212[B]:ARG:HG3	1:C:213:LEU:O	2.19	0.42
1:B:93[B]:SER:OG	3:B:402:3G6:OAF	2.29	0.42
1:D:347:HIS:CE1	1:D:349[A]:VAL:HA	2.54	0.42
1:C:7:VAL:C	1:C:8[A]:GLU:HG2	2.40	0.42
1:D:184:TRP:CH2	1:D:216:ARG:HA	2.54	0.42
1:A:8[B]:GLU:HG2	1:A:40:LYS:HB3	2.02	0.41
1:A:125:ARG:HG3	8:A:804:HOH:O	2.19	0.41
1:C:311:ILE:O	1:C:372:ALA:HA	2.20	0.41
1:D:332:ASP:HB3	1:D:335:ARG:HG3	2.03	0.41
1:D:206:GLN:HA	1:D:207:PRO:HD3	1.94	0.41
1:D:240:HIS:CE1	1:D:320:SER:HB3	2.56	0.41
1:B:136:ARG:HD3	3:B:402:3G6:OAD	2.21	0.41
1:B:17[D]:ARG:CZ	8:B:772:HOH:O	2.68	0.41
3:A:402:3G6:H7	3:A:402:3G6:H16	2.03	0.41
1:C:391[A]:ILE:O	1:C:391[A]:ILE:CG2	2.69	0.40
1:D:347:HIS:CE1	1:D:349[B]:VAL:HA	2.56	0.40
1:A:281:GLY:HA3	1:B:82:GLU:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:NH1	4:D:402[B]:GOL:O3[1_655]	1.81	0.39
1:A:264:ARG:NH1	4:D:402[A]:GOL:O3[1_655]	2.11	0.09
8:C:503:HOH:O	8:D:548:HOH:O[2_446]	2.12	0.08

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	414/399 (104%)	400 (97%)	13 (3%)	1 (0%)	52	32
1	B	404/399 (101%)	395 (98%)	8 (2%)	1 (0%)	52	32
1	C	405/399 (102%)	395 (98%)	10 (2%)	0	100	100
1	D	390/399 (98%)	379 (97%)	11 (3%)	0	100	100
All	All	1613/1596 (101%)	1569 (97%)	42 (3%)	2 (0%)	56	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	B	205	ASN

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	318/303 (105%)	307 (96%)	11 (4%)	43	20
1	B	308/303 (102%)	303 (98%)	5 (2%)	70	54
1	C	311/303 (103%)	306 (98%)	5 (2%)	70	54
1	D	302/303 (100%)	295 (98%)	7 (2%)	58	37
All	All	1239/1212 (102%)	1211 (98%)	28 (2%)	72	37

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	142[A]	GLN
1	A	142[B]	GLN
1	A	178[A]	ARG
1	A	178[B]	ARG
1	A	193	ILE

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Mol	Chain	Res	Type
1	A	211[A]	ARG
1	A	211[B]	ARG
1	A	327[A]	ARG
1	A	327[B]	ARG
1	A	368	ASP
1	B	193	ILE
1	B	212[A]	ARG
1	B	212[B]	ARG
1	B	260[A]	GLU
1	B	260[B]	GLU
1	C	1	MET
1	C	201	LEU
1	C	212[A]	ARG
1	C	212[B]	ARG
1	C	351	CYS
1	D	181[A]	GLN
1	D	181[B]	GLN
1	D	212[A]	ARG
1	D	212[B]	ARG
1	D	221[A]	ARG
1	D	221[B]	ARG
1	D	351	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	92	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)

Of 29 ligands modelled in this entry, 11 are monoatomic - leaving 18 for Mogul analysis.

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	401	-	40,50,50	1.96	8 (20%)	50,75,75	2.08	13 (26%)
3	3G6	A	402	-	25,28,28	1.67	5 (20%)	41,45,45	1.83	10 (24%)
4	GOL	A	403	-	5,5,5	0.36	0	5,5,5	0.27	0
4	GOL	A	404	-	5,5,5	0.33	0	5,5,5	0.22	0
4	GOL	A	405[A]	-	5,5,5	0.35	0	5,5,5	0.22	0
4	GOL	A	405[B]	-	5,5,5	0.31	0	5,5,5	0.26	0
2	COA	B	401[A]	-	40,50,50	1.99	8 (20%)	50,75,75	1.95	8 (16%)
2	COA	B	401[B]	-	40,50,50	1.99	8 (20%)	50,75,75	1.93	8 (16%)
3	3G6	B	402	-	25,28,28	1.69	6 (24%)	41,45,45	1.79	10 (24%)
3	3G6	C	401	-	25,28,28	1.70	5 (20%)	41,45,45	1.86	13 (31%)
2	COA	C	402	-	40,50,50	2.00	10 (25%)	50,75,75	2.01	12 (24%)
4	GOL	C	403[A]	-	5,5,5	0.34	0	5,5,5	0.14	0
4	GOL	C	403[B]	-	5,5,5	0.33	0	5,5,5	0.22	0
6	PEG	C	404	-	6,6,6	0.62	0	5,5,5	0.66	0
2	COA	D	401[A]	-	40,50,50	2.04	11 (27%)	50,75,75	1.99	8 (16%)
2	COA	D	401[B]	-	40,50,50	2.18	11 (27%)	50,75,75	2.68	17 (34%)
4	GOL	D	402[A]	-	5,5,5	0.31	0	5,5,5	0.26	0
4	GOL	D	402[B]	-	5,5,5	0.33	0	5,5,5	0.20	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	401	-	-	0/44/64/64	0/3/3/3
3	3G6	A	402	-	-	0/4/66/66	0/4/4/4
4	GOL	A	403	-	-	0/4/4/4	0/0/0/0
4	GOL	A	404	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	405[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	A	405[B]	-	-	0/4/4/4	0/0/0/0
2	COA	B	401[A]	-	-	0/44/64/64	0/3/3/3
2	COA	B	401[B]	-	-	0/44/64/64	0/3/3/3
3	3G6	B	402	-	-	0/4/66/66	0/4/4/4
3	3G6	C	401	-	-	0/4/66/66	0/4/4/4
2	COA	C	402	-	-	0/44/64/64	0/3/3/3
4	GOL	C	403[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	C	403[B]	-	-	0/4/4/4	0/0/0/0
6	PEG	C	404	-	-	0/4/4/4	0/0/0/0
2	COA	D	401[A]	-	-	0/44/64/64	0/3/3/3
2	COA	D	401[B]	-	-	0/44/64/64	0/3/3/3
4	GOL	D	402[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	D	402[B]	-	-	0/4/4/4	0/0/0/0

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	COA	C2B-C3B	-5.45	1.40	1.53
2	B	401[B]	COA	C2B-C3B	-5.24	1.41	1.53
2	B	401[A]	COA	C2B-C3B	-5.24	1.41	1.53
2	D	401[B]	COA	C2B-C3B	-5.17	1.41	1.53
2	D	401[A]	COA	C2B-C3B	-5.17	1.41	1.53
2	A	401	COA	C2B-C3B	-5.15	1.41	1.53
2	B	401[B]	COA	O4B-C4B	-3.09	1.37	1.45
2	B	401[A]	COA	O4B-C4B	-3.09	1.37	1.45
2	C	402	COA	O4B-C4B	-3.07	1.37	1.45
2	D	401[B]	COA	O4B-C4B	-3.05	1.38	1.45
2	D	401[A]	COA	O4B-C4B	-3.05	1.38	1.45
2	A	401	COA	O4B-C4B	-2.99	1.38	1.45
3	B	402	3G6	CAY-CAW	-2.45	1.50	1.55
3	C	401	3G6	CAB-CAX	-2.42	1.50	1.54
2	B	401[B]	COA	C3B-C4B	-2.42	1.45	1.52
2	B	401[A]	COA	C3B-C4B	-2.42	1.45	1.52
2	D	401[B]	COA	OAP-CAP	-2.42	1.37	1.42
2	D	401[A]	COA	OAP-CAP	-2.42	1.37	1.42
2	D	401[B]	COA	C3B-C4B	-2.39	1.45	1.52
2	D	401[A]	COA	C3B-C4B	-2.39	1.45	1.52
2	A	401	COA	C3B-C4B	-2.39	1.45	1.52
2	C	402	COA	C3B-C4B	-2.38	1.46	1.52
2	A	401	COA	C2P-S1P	-2.37	1.72	1.80
3	C	401	3G6	CAY-CAW	-2.37	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	COA	C2P-S1P	-2.35	1.72	1.80
3	A	402	3G6	CAB-CAX	-2.32	1.50	1.54
3	A	402	3G6	CAN-CAH	-2.31	1.48	1.53
3	B	402	3G6	CAB-CAX	-2.30	1.50	1.54
3	B	402	3G6	CAN-CAH	-2.29	1.48	1.53
2	B	401[A]	COA	C2P-S1P	-2.28	1.73	1.80
2	C	402	COA	C2P-S1P	-2.23	1.73	1.80
3	A	402	3G6	CAY-CAW	-2.21	1.50	1.55
3	C	401	3G6	CAN-CAH	-2.19	1.48	1.53
2	D	401[B]	COA	O9P-C9P	-2.17	1.19	1.23
2	D	401[A]	COA	O9P-C9P	-2.17	1.19	1.23
3	B	402	3G6	CAO-CAY	-2.15	1.50	1.54
2	D	401[A]	COA	C2P-S1P	-2.10	1.73	1.80
2	C	402	COA	OAP-CAP	-2.05	1.38	1.42
2	C	402	COA	O9P-C9P	-2.04	1.19	1.23
2	D	401[B]	COA	C2A-N3A	2.02	1.35	1.32
2	D	401[A]	COA	C2A-N3A	2.02	1.35	1.32
2	C	402	COA	C4A-N3A	2.11	1.38	1.35
2	B	401[B]	COA	C4A-N3A	2.18	1.38	1.35
2	B	401[A]	COA	C4A-N3A	2.18	1.38	1.35
2	D	401[B]	COA	C6P-C5P	2.22	1.55	1.51
2	A	401	COA	C4A-N3A	2.23	1.38	1.35
2	D	401[B]	COA	C4A-N3A	2.34	1.39	1.35
2	D	401[A]	COA	C4A-N3A	2.34	1.39	1.35
3	C	401	3G6	CAI-CAR	2.86	1.55	1.50
3	B	402	3G6	CAI-CAR	2.97	1.55	1.50
3	A	402	3G6	CAI-CAR	3.11	1.55	1.50
2	A	401	COA	C6A-N6A	3.73	1.46	1.34
2	C	402	COA	C6A-N6A	3.83	1.46	1.34
2	B	401[B]	COA	C6A-N6A	3.93	1.47	1.34
2	B	401[A]	COA	C6A-N6A	3.93	1.47	1.34
2	D	401[B]	COA	C6A-N6A	3.95	1.47	1.34
2	D	401[A]	COA	C6A-N6A	3.95	1.47	1.34
3	B	402	3G6	CAG-CAR	4.35	1.40	1.34
3	A	402	3G6	CAG-CAR	4.35	1.40	1.34
3	C	401	3G6	CAG-CAR	4.38	1.40	1.34
2	A	401	COA	C5P-N4P	4.68	1.44	1.33
2	D	401[A]	COA	C5P-N4P	4.74	1.44	1.33
2	C	402	COA	C5P-N4P	4.78	1.44	1.33
2	B	401[B]	COA	C5P-N4P	4.79	1.44	1.33
2	B	401[A]	COA	C5P-N4P	4.85	1.45	1.33
2	D	401[B]	COA	C5P-N4P	5.63	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	COA	C9P-N8P	6.01	1.46	1.33
2	A	401	COA	C9P-N8P	6.04	1.46	1.33
2	B	401[B]	COA	C9P-N8P	6.20	1.46	1.33
2	B	401[A]	COA	C9P-N8P	6.20	1.46	1.33
2	D	401[A]	COA	C9P-N8P	6.52	1.47	1.33
2	D	401[B]	COA	C9P-N8P	7.32	1.48	1.33

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401[B]	COA	N3A-C2A-N1A	-10.48	120.87	128.89
2	D	401[A]	COA	N3A-C2A-N1A	-10.48	120.87	128.89
2	A	401	COA	N3A-C2A-N1A	-10.35	120.97	128.89
2	B	401[B]	COA	N3A-C2A-N1A	-10.04	121.21	128.89
2	B	401[A]	COA	N3A-C2A-N1A	-10.04	121.21	128.89
2	C	402	COA	N3A-C2A-N1A	-9.79	121.40	128.89
2	D	401[B]	COA	O9P-C9P-N8P	-4.96	113.13	123.08
3	C	401	3G6	CAV-CAY-CAW	-4.18	95.18	100.09
3	A	402	3G6	CAX-CAR-CAG	-4.08	118.04	122.69
2	D	401[B]	COA	P2A-O3A-P1A	-3.77	122.14	132.73
2	D	401[A]	COA	P2A-O3A-P1A	-3.77	122.14	132.73
3	B	402	3G6	CAN-CAX-CAU	-3.70	103.89	108.64
3	A	402	3G6	CAN-CAX-CAU	-3.59	104.03	108.64
2	C	402	COA	C7P-N8P-C9P	-3.53	115.54	122.53
2	D	401[B]	COA	C7P-N8P-C9P	-3.50	115.60	122.53
2	D	401[B]	COA	O5P-C5P-C6P	-3.30	116.29	121.98
2	B	401[B]	COA	OAP-CAP-C9P	-3.28	102.85	110.38
2	B	401[A]	COA	OAP-CAP-C9P	-3.28	102.85	110.38
3	B	402	3G6	CAV-CAY-CAW	-3.23	96.29	100.09
3	C	401	3G6	CAN-CAX-CAU	-3.21	104.52	108.64
3	B	402	3G6	CAX-CAR-CAG	-3.17	119.08	122.69
2	D	401[B]	COA	O5P-C5P-N4P	-3.17	116.65	122.94
3	C	401	3G6	CAX-CAR-CAG	-3.12	119.14	122.69
3	A	402	3G6	CAV-CAY-CAW	-3.05	96.51	100.09
2	B	401[B]	COA	C7P-C6P-C5P	-2.91	107.52	112.31
2	B	401[A]	COA	C7P-C6P-C5P	-2.91	107.52	112.31
2	C	402	COA	P2A-O3A-P1A	-2.79	124.89	132.73
2	A	401	COA	C2P-C3P-N4P	-2.78	106.88	112.37
2	A	401	COA	OAP-CAP-C9P	-2.76	104.05	110.38
2	A	401	COA	C1B-N9A-C4A	-2.76	122.78	126.94
2	A	401	COA	C3P-N4P-C5P	-2.61	117.66	122.79
2	A	401	COA	C7P-N8P-C9P	-2.53	117.52	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	402	COA	C3P-N4P-C5P	-2.51	117.84	122.79
2	C	402	COA	C1B-N9A-C4A	-2.51	123.15	126.94
2	D	401[B]	COA	OAP-CAP-C9P	-2.49	104.66	110.38
2	D	401[A]	COA	OAP-CAP-C9P	-2.49	104.66	110.38
2	C	402	COA	OAP-CAP-C9P	-2.47	104.70	110.38
2	A	401	COA	P2A-O3A-P1A	-2.47	125.79	132.73
3	A	402	3G6	CAK-CAV-CAS	-2.46	108.02	111.86
2	B	401[A]	COA	C3P-N4P-C5P	-2.42	118.03	122.79
2	B	401[B]	COA	P2A-O3A-P1A	-2.36	126.09	132.73
2	B	401[A]	COA	P2A-O3A-P1A	-2.36	126.09	132.73
2	A	401	COA	C7P-C6P-C5P	-2.36	108.43	112.31
2	D	401[B]	COA	C4A-C5A-N7A	-2.35	107.31	109.48
2	D	401[A]	COA	C4A-C5A-N7A	-2.35	107.31	109.48
3	C	401	3G6	CAK-CAV-CAS	-2.34	108.20	111.86
2	B	401[B]	COA	C4A-C5A-N7A	-2.28	107.38	109.48
2	B	401[A]	COA	C4A-C5A-N7A	-2.28	107.38	109.48
2	C	402	COA	C7P-C6P-C5P	-2.27	108.58	112.31
3	B	402	3G6	CAR-CAG-CAP	-2.26	120.63	123.75
2	A	401	COA	C4A-C5A-N7A	-2.23	107.43	109.48
3	A	402	3G6	CAR-CAG-CAP	-2.23	120.68	123.75
2	B	401[B]	COA	C3P-N4P-C5P	-2.23	118.41	122.79
3	A	402	3G6	OAD-CAP-CAH	-2.22	118.26	121.60
3	B	402	3G6	CAU-CAX-CAR	-2.18	106.29	109.67
3	C	401	3G6	CAR-CAG-CAP	-2.14	120.79	123.75
3	B	402	3G6	CAY-CAV-CAS	-2.14	116.36	119.23
2	C	402	COA	O5P-C5P-C6P	-2.13	118.31	121.98
2	C	402	COA	C4A-C5A-N7A	-2.05	107.59	109.48
2	D	401[B]	COA	C1B-N9A-C4A	-2.03	123.88	126.94
2	D	401[A]	COA	C1B-N9A-C4A	-2.03	123.88	126.94
3	C	401	3G6	CAA-CAS-CAQ	-2.01	105.60	111.81
3	C	401	3G6	CAX-CAU-CAT	2.00	115.63	112.67
2	B	401[B]	COA	C6P-C5P-N4P	2.03	119.99	116.46
3	C	401	3G6	CAM-CAU-CAX	2.03	115.81	113.11
3	C	401	3G6	CAK-CAV-CAY	2.05	106.48	103.82
2	B	401[B]	COA	C6P-C7P-N8P	2.06	116.40	111.88
2	B	401[A]	COA	C6P-C7P-N8P	2.06	116.40	111.88
2	A	401	COA	O4B-C1B-N9A	2.07	112.43	108.10
2	D	401[A]	COA	C6P-C7P-N8P	2.08	116.44	111.88
3	B	402	3G6	CAK-CAV-CAY	2.09	106.54	103.82
2	D	401[B]	COA	O3A-P1A-O5B	2.11	108.53	102.94
2	D	401[A]	COA	O3A-P1A-O5B	2.11	108.53	102.94
2	A	401	COA	CEP-CBP-CCP	2.15	111.28	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	3G6	CAB-CAX-CAU	2.23	114.51	111.67
3	C	401	3G6	CAM-CAO-CAY	2.35	117.04	112.84
2	A	401	COA	C6P-C7P-N8P	2.36	117.05	111.88
2	C	402	COA	O4B-C1B-N9A	2.37	113.06	108.10
3	A	402	3G6	CAC-CAY-CAW	2.39	116.43	111.75
2	D	401[B]	COA	C2P-C3P-N4P	2.42	117.14	112.37
2	C	402	COA	C6P-C5P-N4P	2.51	120.81	116.46
2	C	402	COA	C6P-C7P-N8P	2.52	117.40	111.88
3	C	401	3G6	CAC-CAY-CAW	2.52	116.69	111.75
3	A	402	3G6	CAX-CAU-CAT	2.52	116.40	112.67
2	B	401[A]	COA	C6P-C5P-N4P	2.54	120.87	116.46
2	D	401[B]	COA	C3P-N4P-C5P	2.82	128.33	122.79
2	A	401	COA	O3A-P1A-O5B	2.88	110.59	102.94
3	C	401	3G6	CAH-CAP-CAG	3.02	121.34	116.70
3	B	402	3G6	CAH-CAP-CAG	3.13	121.51	116.70
2	D	401[B]	COA	C7P-C6P-C5P	3.30	117.75	112.31
3	A	402	3G6	CAH-CAP-CAG	3.32	121.81	116.70
2	D	401[B]	COA	O6A-CCP-CBP	3.40	116.01	110.55
2	D	401[A]	COA	O6A-CCP-CBP	3.40	116.01	110.55
3	B	402	3G6	CAI-CAR-CAX	3.99	121.24	116.71
3	C	401	3G6	CAI-CAR-CAX	4.39	121.70	116.71
3	A	402	3G6	CAI-CAR-CAX	4.68	122.03	116.71
2	D	401[B]	COA	CAP-C9P-N8P	4.89	127.31	116.47
2	D	401[B]	COA	C6P-C7P-N8P	5.74	124.48	111.88
2	D	401[B]	COA	C6P-C5P-N4P	6.10	127.06	116.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	3G6	2	0
3	B	402	3G6	5	0
3	C	401	3G6	1	0
6	C	404	PEG	1	0
4	D	402[A]	GOL	0	1
4	D	402[B]	GOL	1	1

5.7 Other polymers

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, 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	396/399 (99%)	0.16	26 (6%)	22	23	15, 25, 52, 83	3 (0%)
1	B	392/399 (98%)	0.16	20 (5%)	32	34	14, 26, 50, 85	0
1	C	391/399 (97%)	0.13	18 (4%)	36	40	16, 28, 56, 107	0
1	D	376/399 (94%)	0.16	18 (4%)	34	38	15, 25, 51, 113	0
All	All	1555/1596 (97%)	0.15	82 (5%)	30	32	14, 26, 52, 113	3 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	GLU	7.0
1	A	-1	GLY	6.3
1	D	204	GLN	5.8
1	A	44	GLN	5.6
1	A	-3	HIS	5.5
1	A	43	ILE	5.5
1	D	208	THR	4.9
1	D	201	LEU	4.9
1	D	203	GLU	4.5
1	C	134	PRO	4.0
1	A	46	GLY	4.0
1	D	1	MET	4.0
1	C	204	GLN	3.8
1	C	201	LEU	3.8
1	B	202	ASP	3.8
1	B	205	ASN	3.7
1	C	202[A]	ASP	3.7
1	D	207	PRO	3.6
1	C	89	VAL	3.4
1	D	205	ASN	3.3
1	C	391[A]	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	210[A]	GLU	3.3
1	B	201	LEU	3.3
1	A	265	ALA	3.2
1	C	102	LEU	3.2
1	A	203	GLU	3.2
1	D	206	GLN	3.1
1	A	-2	HIS	3.1
1	D	202	ASP	3.0
1	A	45	SER	3.0
1	B	204	GLN	2.9
1	C	142[A]	GLN	2.9
1	A	135[A]	ASP	2.9
1	B	89	VAL	2.9
1	C	205	ASN	2.8
1	D	212[A]	ARG	2.8
1	B	200	VAL	2.8
1	C	3	TYR	2.8
1	C	135	ASP	2.8
1	D	89	VAL	2.7
1	A	206	GLN	2.7
1	A	279	LEU	2.7
1	D	44	GLN	2.7
1	A	89	VAL	2.7
1	B	1	MET	2.6
1	C	137	SER	2.6
1	B	56	ILE	2.6
1	A	142[A]	GLN	2.6
1	A	382	LEU	2.5
1	A	-4	HIS	2.5
1	D	3	TYR	2.5
1	B	206	GLN	2.5
1	B	86	ALA	2.5
1	D	56	ILE	2.5
1	C	232	LYS	2.5
1	D	234	VAL	2.4
1	A	56	ILE	2.4
1	A	391	ILE	2.4
1	A	134[A]	PRO	2.4
1	B	84	VAL	2.4
1	B	210	GLU	2.4
1	A	48[A]	HIS	2.4
1	B	237	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	206	GLN	2.3
1	B	207	PRO	2.3
1	A	47	LEU	2.3
1	A	42	GLY	2.3
1	D	102	LEU	2.3
1	B	203	GLU	2.3
1	A	91	CYS	2.3
1	B	0	SER	2.3
1	C	200	VAL	2.2
1	C	212[A]	ARG	2.2
1	A	268	LEU	2.1
1	D	99	ALA	2.1
1	B	91	CYS	2.1
1	B	209	GLY	2.1
1	A	266	HIS	2.1
1	C	58	GLY	2.1
1	B	116	ILE	2.0
1	A	0	SER	2.0
1	B	87	THR	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
5	CL	D	403	1/1	0.94	0.21	8.98	62,62,62,62	0
4	GOL	A	405[A]	6/6	0.54	0.29	7.13	69,70,73,73	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	405[B]	6/6	0.54	0.29	7.13	70,73,74,79	6
4	GOL	C	403[B]	6/6	0.83	0.13	7.03	47,52,52,52	6
4	GOL	C	403[A]	6/6	0.83	0.13	7.03	48,50,52,53	6
4	GOL	D	402[A]	6/6	0.82	0.34	6.65	57,58,60,63	6
4	GOL	D	402[B]	6/6	0.82	0.34	6.28	56,58,60,63	6
4	GOL	A	403	6/6	0.85	0.27	4.17	64,67,69,71	0
6	PEG	C	404	7/7	0.77	0.30	4.04	54,58,62,62	0
2	COA	D	401[A]	48/48	0.81	0.23	3.02	29,49,78,80	24
2	COA	D	401[B]	48/48	0.81	0.23	3.02	29,49,78,80	24
3	3G6	B	402	25/25	0.86	0.17	2.78	28,38,57,64	0
2	COA	C	402	48/48	0.89	0.16	1.87	30,41,145,148	0
4	GOL	A	404	6/6	0.84	0.14	1.85	35,46,47,48	0
2	COA	A	401	48/48	0.92	0.15	1.51	23,36,153,156	0
2	COA	B	401[B]	48/48	0.94	0.11	1.33	26,35,147,150	4
5	CL	A	407	1/1	0.93	0.22	0.79	67,67,67,67	0
2	COA	B	401[A]	48/48	0.94	0.11	0.77	26,35,147,150	4
3	3G6	A	402	25/25	0.89	0.11	0.35	21,30,49,60	0
3	3G6	C	401	25/25	0.88	0.11	0.15	29,42,61,68	0
5	CL	B	405	1/1	0.97	0.20	0.11	67,67,67,67	0
7	NA	C	406	1/1	0.82	0.09	-0.42	56,56,56,56	0
5	CL	B	407	1/1	0.90	0.06	-2.07	74,74,74,74	0
5	CL	D	404	1/1	0.99	0.06	-2.58	35,35,35,35	0
5	CL	A	406	1/1	0.87	0.19	-	74,74,74,74	0
5	CL	C	405	1/1	0.90	0.30	-	65,65,65,65	0
5	CL	B	403	1/1	0.93	0.29	-	60,60,60,60	0
5	CL	B	406	1/1	0.91	0.09	-	78,78,78,78	0
5	CL	B	404	1/1	0.91	0.07	-	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.