Full wwPDB X-ray Structure Validation Report

Dec 18, 2016 – 04:55 AM EST

PDB ID	:	5THQ
Title	:	Comprehensive Analysis of a Novel Ketoreductase for Pentangular Polyphenol Biosynthesis
Authors	:	Valentic, T.R.; Tsai, S.C.; Brady, S.F.
Deposited on	:	2016-09-30
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the symbol.

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

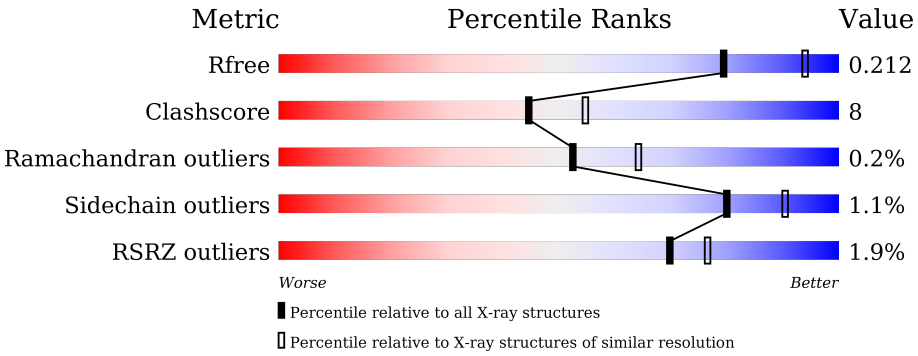
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	272	85% 6% 9%
1	B	272	79% 13% 8%
1	C	272	3% 77% 14% • 8%
1	D	272	81% 10% • 8%
1	E	272	2% 78% 14% 8%
1	F	272	3% 76% 15% • 8%

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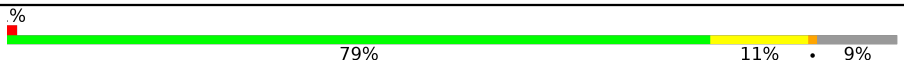
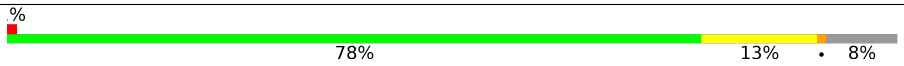
Mol	Chain	Length	Quality of chain
1	G	272	
1	H	272	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15849 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-oxoacyl-ACP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	248	Total	C	N	O	S	0	0	0
			1858	1166	341	349	2			
1	B	250	Total	C	N	O	S	0	0	0
			1875	1177	343	353	2			
1	C	250	Total	C	N	O	S	0	0	0
			1875	1177	343	353	2			
1	F	250	Total	C	N	O	S	0	0	0
			1875	1177	343	353	2			
1	A	248	Total	C	N	O	S	0	0	0
			1858	1166	341	349	2			
1	E	250	Total	C	N	O	S	0	0	0
			1875	1177	343	353	2			
1	H	250	Total	C	N	O	S	0	0	0
			1875	1177	343	353	2			
1	D	250	Total	C	N	O	S	0	0	0
			1875	1177	343	353	2			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	initiating methionine	UNP A0A023PKG5
G	-18	GLY	-	expression tag	UNP A0A023PKG5
G	-17	SER	-	expression tag	UNP A0A023PKG5
G	-16	SER	-	expression tag	UNP A0A023PKG5
G	-15	HIS	-	expression tag	UNP A0A023PKG5
G	-14	HIS	-	expression tag	UNP A0A023PKG5
G	-13	HIS	-	expression tag	UNP A0A023PKG5
G	-12	HIS	-	expression tag	UNP A0A023PKG5
G	-11	HIS	-	expression tag	UNP A0A023PKG5
G	-10	HIS	-	expression tag	UNP A0A023PKG5
G	-9	SER	-	expression tag	UNP A0A023PKG5
G	-8	SER	-	expression tag	UNP A0A023PKG5
G	-7	GLY	-	expression tag	UNP A0A023PKG5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	LEU	-	expression tag	UNP A0A023PKG5
G	-5	VAL	-	expression tag	UNP A0A023PKG5
G	-4	PRO	-	expression tag	UNP A0A023PKG5
G	-3	ARG	-	expression tag	UNP A0A023PKG5
G	-2	GLY	-	expression tag	UNP A0A023PKG5
G	-1	SER	-	expression tag	UNP A0A023PKG5
G	0	HIS	-	expression tag	UNP A0A023PKG5
B	-19	MET	-	initiating methionine	UNP A0A023PKG5
B	-18	GLY	-	expression tag	UNP A0A023PKG5
B	-17	SER	-	expression tag	UNP A0A023PKG5
B	-16	SER	-	expression tag	UNP A0A023PKG5
B	-15	HIS	-	expression tag	UNP A0A023PKG5
B	-14	HIS	-	expression tag	UNP A0A023PKG5
B	-13	HIS	-	expression tag	UNP A0A023PKG5
B	-12	HIS	-	expression tag	UNP A0A023PKG5
B	-11	HIS	-	expression tag	UNP A0A023PKG5
B	-10	HIS	-	expression tag	UNP A0A023PKG5
B	-9	SER	-	expression tag	UNP A0A023PKG5
B	-8	SER	-	expression tag	UNP A0A023PKG5
B	-7	GLY	-	expression tag	UNP A0A023PKG5
B	-6	LEU	-	expression tag	UNP A0A023PKG5
B	-5	VAL	-	expression tag	UNP A0A023PKG5
B	-4	PRO	-	expression tag	UNP A0A023PKG5
B	-3	ARG	-	expression tag	UNP A0A023PKG5
B	-2	GLY	-	expression tag	UNP A0A023PKG5
B	-1	SER	-	expression tag	UNP A0A023PKG5
B	0	HIS	-	expression tag	UNP A0A023PKG5
C	-19	MET	-	initiating methionine	UNP A0A023PKG5
C	-18	GLY	-	expression tag	UNP A0A023PKG5
C	-17	SER	-	expression tag	UNP A0A023PKG5
C	-16	SER	-	expression tag	UNP A0A023PKG5
C	-15	HIS	-	expression tag	UNP A0A023PKG5
C	-14	HIS	-	expression tag	UNP A0A023PKG5
C	-13	HIS	-	expression tag	UNP A0A023PKG5
C	-12	HIS	-	expression tag	UNP A0A023PKG5
C	-11	HIS	-	expression tag	UNP A0A023PKG5
C	-10	HIS	-	expression tag	UNP A0A023PKG5
C	-9	SER	-	expression tag	UNP A0A023PKG5
C	-8	SER	-	expression tag	UNP A0A023PKG5
C	-7	GLY	-	expression tag	UNP A0A023PKG5
C	-6	LEU	-	expression tag	UNP A0A023PKG5
C	-5	VAL	-	expression tag	UNP A0A023PKG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A023PKG5
C	-3	ARG	-	expression tag	UNP A0A023PKG5
C	-2	GLY	-	expression tag	UNP A0A023PKG5
C	-1	SER	-	expression tag	UNP A0A023PKG5
C	0	HIS	-	expression tag	UNP A0A023PKG5
F	-19	MET	-	initiating methionine	UNP A0A023PKG5
F	-18	GLY	-	expression tag	UNP A0A023PKG5
F	-17	SER	-	expression tag	UNP A0A023PKG5
F	-16	SER	-	expression tag	UNP A0A023PKG5
F	-15	HIS	-	expression tag	UNP A0A023PKG5
F	-14	HIS	-	expression tag	UNP A0A023PKG5
F	-13	HIS	-	expression tag	UNP A0A023PKG5
F	-12	HIS	-	expression tag	UNP A0A023PKG5
F	-11	HIS	-	expression tag	UNP A0A023PKG5
F	-10	HIS	-	expression tag	UNP A0A023PKG5
F	-9	SER	-	expression tag	UNP A0A023PKG5
F	-8	SER	-	expression tag	UNP A0A023PKG5
F	-7	GLY	-	expression tag	UNP A0A023PKG5
F	-6	LEU	-	expression tag	UNP A0A023PKG5
F	-5	VAL	-	expression tag	UNP A0A023PKG5
F	-4	PRO	-	expression tag	UNP A0A023PKG5
F	-3	ARG	-	expression tag	UNP A0A023PKG5
F	-2	GLY	-	expression tag	UNP A0A023PKG5
F	-1	SER	-	expression tag	UNP A0A023PKG5
F	0	HIS	-	expression tag	UNP A0A023PKG5
A	-19	MET	-	initiating methionine	UNP A0A023PKG5
A	-18	GLY	-	expression tag	UNP A0A023PKG5
A	-17	SER	-	expression tag	UNP A0A023PKG5
A	-16	SER	-	expression tag	UNP A0A023PKG5
A	-15	HIS	-	expression tag	UNP A0A023PKG5
A	-14	HIS	-	expression tag	UNP A0A023PKG5
A	-13	HIS	-	expression tag	UNP A0A023PKG5
A	-12	HIS	-	expression tag	UNP A0A023PKG5
A	-11	HIS	-	expression tag	UNP A0A023PKG5
A	-10	HIS	-	expression tag	UNP A0A023PKG5
A	-9	SER	-	expression tag	UNP A0A023PKG5
A	-8	SER	-	expression tag	UNP A0A023PKG5
A	-7	GLY	-	expression tag	UNP A0A023PKG5
A	-6	LEU	-	expression tag	UNP A0A023PKG5
A	-5	VAL	-	expression tag	UNP A0A023PKG5
A	-4	PRO	-	expression tag	UNP A0A023PKG5
A	-3	ARG	-	expression tag	UNP A0A023PKG5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A023PKG5
A	-1	SER	-	expression tag	UNP A0A023PKG5
A	0	HIS	-	expression tag	UNP A0A023PKG5
E	-19	MET	-	initiating methionine	UNP A0A023PKG5
E	-18	GLY	-	expression tag	UNP A0A023PKG5
E	-17	SER	-	expression tag	UNP A0A023PKG5
E	-16	SER	-	expression tag	UNP A0A023PKG5
E	-15	HIS	-	expression tag	UNP A0A023PKG5
E	-14	HIS	-	expression tag	UNP A0A023PKG5
E	-13	HIS	-	expression tag	UNP A0A023PKG5
E	-12	HIS	-	expression tag	UNP A0A023PKG5
E	-11	HIS	-	expression tag	UNP A0A023PKG5
E	-10	HIS	-	expression tag	UNP A0A023PKG5
E	-9	SER	-	expression tag	UNP A0A023PKG5
E	-8	SER	-	expression tag	UNP A0A023PKG5
E	-7	GLY	-	expression tag	UNP A0A023PKG5
E	-6	LEU	-	expression tag	UNP A0A023PKG5
E	-5	VAL	-	expression tag	UNP A0A023PKG5
E	-4	PRO	-	expression tag	UNP A0A023PKG5
E	-3	ARG	-	expression tag	UNP A0A023PKG5
E	-2	GLY	-	expression tag	UNP A0A023PKG5
E	-1	SER	-	expression tag	UNP A0A023PKG5
E	0	HIS	-	expression tag	UNP A0A023PKG5
H	-19	MET	-	initiating methionine	UNP A0A023PKG5
H	-18	GLY	-	expression tag	UNP A0A023PKG5
H	-17	SER	-	expression tag	UNP A0A023PKG5
H	-16	SER	-	expression tag	UNP A0A023PKG5
H	-15	HIS	-	expression tag	UNP A0A023PKG5
H	-14	HIS	-	expression tag	UNP A0A023PKG5
H	-13	HIS	-	expression tag	UNP A0A023PKG5
H	-12	HIS	-	expression tag	UNP A0A023PKG5
H	-11	HIS	-	expression tag	UNP A0A023PKG5
H	-10	HIS	-	expression tag	UNP A0A023PKG5
H	-9	SER	-	expression tag	UNP A0A023PKG5
H	-8	SER	-	expression tag	UNP A0A023PKG5
H	-7	GLY	-	expression tag	UNP A0A023PKG5
H	-6	LEU	-	expression tag	UNP A0A023PKG5
H	-5	VAL	-	expression tag	UNP A0A023PKG5
H	-4	PRO	-	expression tag	UNP A0A023PKG5
H	-3	ARG	-	expression tag	UNP A0A023PKG5
H	-2	GLY	-	expression tag	UNP A0A023PKG5
H	-1	SER	-	expression tag	UNP A0A023PKG5

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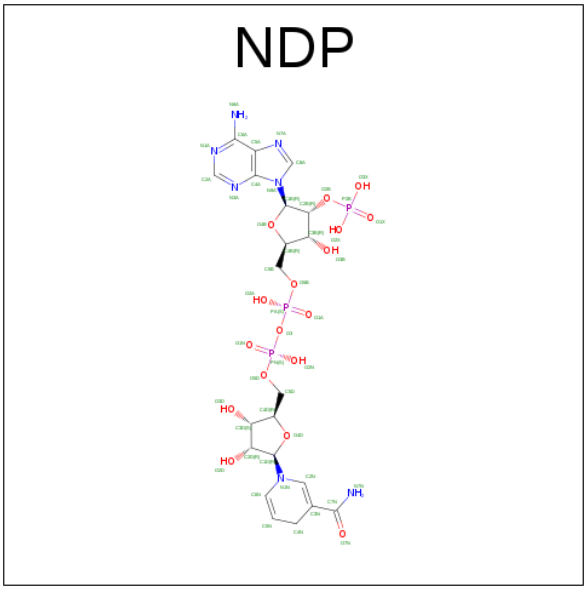
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP A0A023PKG5
D	-19	MET	-	initiating methionine	UNP A0A023PKG5
D	-18	GLY	-	expression tag	UNP A0A023PKG5
D	-17	SER	-	expression tag	UNP A0A023PKG5
D	-16	SER	-	expression tag	UNP A0A023PKG5
D	-15	HIS	-	expression tag	UNP A0A023PKG5
D	-14	HIS	-	expression tag	UNP A0A023PKG5
D	-13	HIS	-	expression tag	UNP A0A023PKG5
D	-12	HIS	-	expression tag	UNP A0A023PKG5
D	-11	HIS	-	expression tag	UNP A0A023PKG5
D	-10	HIS	-	expression tag	UNP A0A023PKG5
D	-9	SER	-	expression tag	UNP A0A023PKG5
D	-8	SER	-	expression tag	UNP A0A023PKG5
D	-7	GLY	-	expression tag	UNP A0A023PKG5
D	-6	LEU	-	expression tag	UNP A0A023PKG5
D	-5	VAL	-	expression tag	UNP A0A023PKG5
D	-4	PRO	-	expression tag	UNP A0A023PKG5
D	-3	ARG	-	expression tag	UNP A0A023PKG5
D	-2	GLY	-	expression tag	UNP A0A023PKG5
D	-1	SER	-	expression tag	UNP A0A023PKG5
D	0	HIS	-	expression tag	UNP A0A023PKG5

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

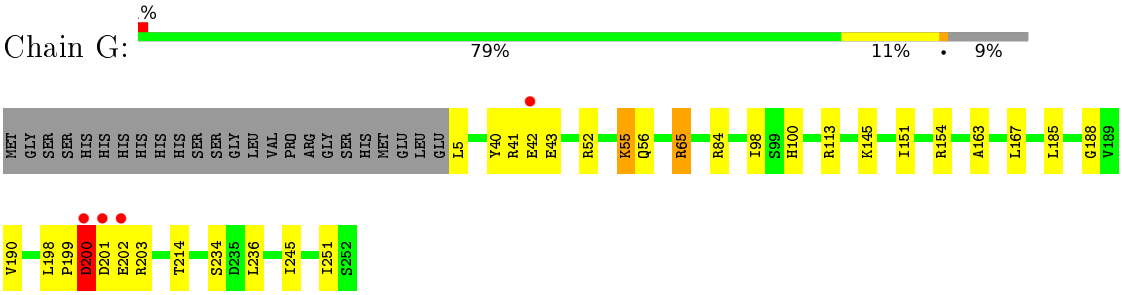
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	54	Total	O	0	0
			54	54		
3	B	60	Total	O	0	0
			60	60		
3	C	36	Total	O	0	0
			36	36		
3	F	49	Total	O	0	0
			49	49		
3	A	80	Total	O	0	0
			80	80		
3	E	65	Total	O	0	0
			65	65		
3	H	77	Total	O	0	0
			77	77		
3	D	78	Total	O	0	0
			78	78		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

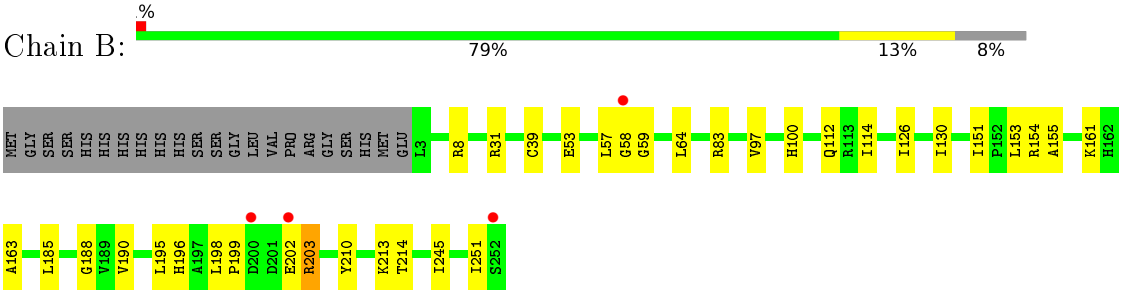
- Molecule 1: 3-oxoacyl-ACP reductase

Chain G:



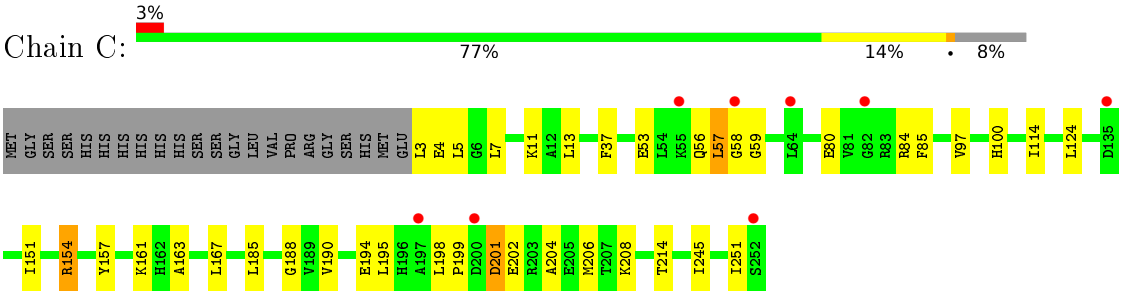
- Molecule 1: 3-oxoacyl-ACP reductase

Chain B:



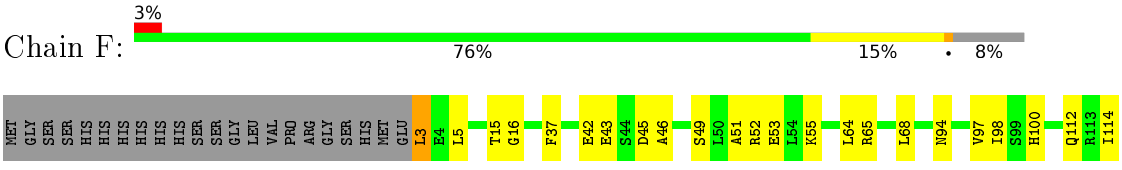
- Molecule 1: 3-oxoacyl-ACP reductase

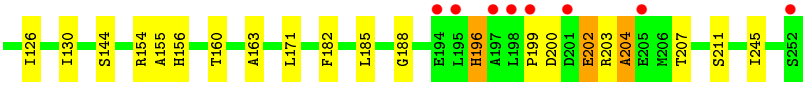
Chain C:



- Molecule 1: 3-oxoacyl-ACP reductase

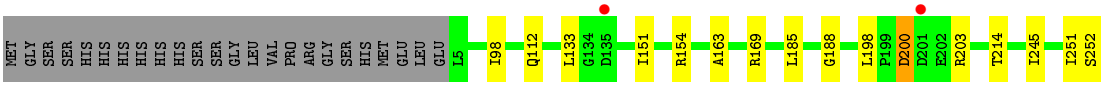
Chain F:





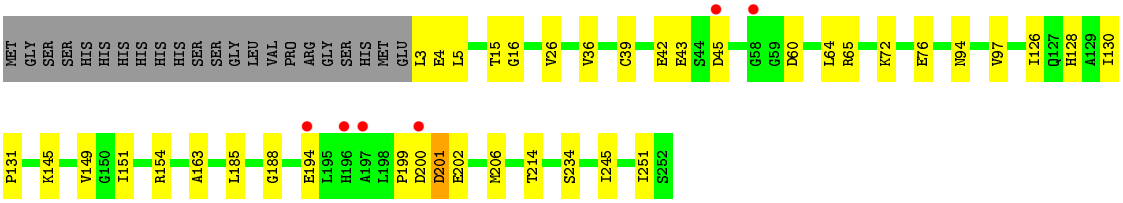
• Molecule 1: 3-oxoacyl-ACP reductase

Chain A:



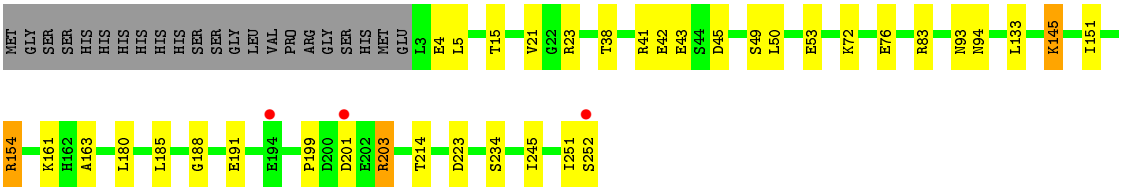
• Molecule 1: 3-oxoacyl-ACP reductase

Chain E:



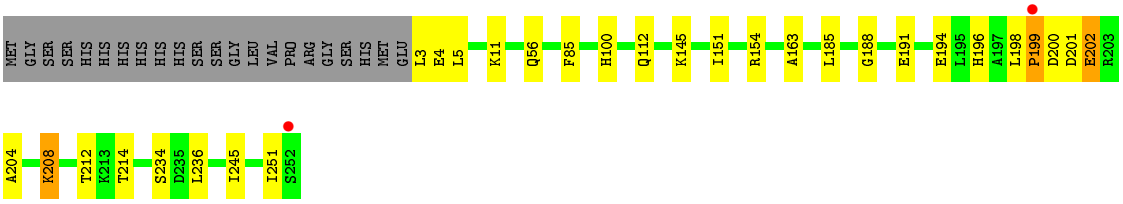
• Molecule 1: 3-oxoacyl-ACP reductase

Chain H:



• Molecule 1: 3-oxoacyl-ACP 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	105.34Å 86.54Å 106.97Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	86.31 – 2.30 86.30 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (86.31-2.30) 94.2 (86.30-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.169 , 0.217 0.162 , 0.212	Depositor DCC
R_{free} test set	1907 reflections (2.50%)	DCC
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15849	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.49 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.7940e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

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	0.48	0/1888	0.74	2/2558 (0.1%)
1	B	0.48	0/1905	0.76	1/2581 (0.0%)
1	C	0.44	0/1905	0.69	1/2581 (0.0%)
1	D	0.51	0/1905	0.70	0/2581
1	E	0.53	1/1905 (0.1%)	0.72	0/2581
1	F	0.50	0/1905	0.71	0/2581
1	G	0.53	0/1888	0.77	4/2558 (0.2%)
1	H	0.66	4/1905 (0.2%)	0.72	0/2581
All	All	0.52	5/15206 (0.0%)	0.73	8/20602 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	1
1	F	0	2
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	203	ARG	CZ-NH2	-10.45	1.19	1.33
1	H	203	ARG	NE-CZ	-9.78	1.20	1.33
1	H	203	ARG	CD-NE	-7.60	1.33	1.46
1	H	203	ARG	CZ-NH1	-7.55	1.23	1.33
1	E	194	GLU	CD-OE2	5.30	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	G	84	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	169	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	G	65	ARG	CG-CD-NE	-7.26	96.55	111.80
1	G	84	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	169	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	G	200	ASP	CB-CA-C	-5.81	98.78	110.40
1	C	57	LEU	CA-CB-CG	5.48	127.90	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	194	GLU	Sidechain
1	C	201	ASP	Peptide
1	D	199	PRO	Peptide
1	F	202	GLU	Peptide
1	F	204	ALA	Peptide

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	1858	0	1886	14	0
1	B	1875	0	1903	31	0
1	C	1875	0	1903	41	0
1	D	1875	0	1903	27	0
1	E	1875	0	1903	31	1
1	F	1875	0	1903	51	0
1	G	1858	0	1886	33	0
1	H	1875	0	1903	24	1
2	A	48	0	25	1	0
2	B	48	0	24	2	0
2	C	48	0	25	2	0
2	D	48	0	25	1	0
2	E	48	0	25	6	0
2	F	48	0	25	9	0
2	G	48	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	48	0	26	3	0
3	A	80	0	0	2	0
3	B	60	0	0	12	0
3	C	36	0	0	5	0
3	D	78	0	0	6	0
3	E	65	0	0	3	0
3	F	49	0	0	4	0
3	G	54	0	0	3	0
3	H	77	0	0	6	0
All	All	15849	0	15390	242	1

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 (242) 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:F:49:SER:HB3	3:F:402:HOH:O	1.25	1.30
1:B:53:GLU:HB2	3:B:401:HOH:O	1.29	1.30
1:D:3:LEU:N	3:D:401:HOH:O	1.85	1.09
1:G:151:ILE:HB	1:G:154:ARG:NH1	1.68	1.08
1:C:58:GLY:C	3:C:401:HOH:O	1.93	1.05
1:C:151:ILE:HG21	1:C:154:ARG:NH1	1.73	1.03
1:G:42:GLU:HA	1:G:65:ARG:HH12	1.21	1.01
1:G:41:ARG:O	1:G:65:ARG:NH1	1.96	0.98
1:H:23:ARG:NH2	1:H:53:GLU:OE1	1.96	0.98
1:B:58:GLY:C	3:B:402:HOH:O	2.03	0.96
1:D:3:LEU:CA	3:D:401:HOH:O	2.10	0.96
2:H:301:NDP:O2N	3:H:401:HOH:O	1.84	0.94
1:F:204:ALA:HB1	1:F:207:THR:H	1.34	0.92
1:G:42:GLU:CA	1:G:65:ARG:HH12	1.81	0.92
1:H:41:ARG:NH2	1:H:42:GLU:OE2	2.04	0.90
1:G:198:LEU:O	1:G:203:ARG:NH1	2.04	0.90
1:A:98:ILE:HD11	1:A:154:ARG:HD3	1.54	0.90
1:C:57:LEU:O	3:C:401:HOH:O	1.92	0.87
1:C:201:ASP:HA	1:C:204:ALA:H	1.41	0.86
1:B:53:GLU:OE1	3:B:401:HOH:O	1.92	0.86
1:D:3:LEU:HA	3:D:401:HOH:O	1.74	0.85
1:B:59:GLY:N	3:B:402:HOH:O	2.11	0.83
1:F:16:GLY:HA2	2:F:301:NDP:H1B	1.62	0.82
1:F:45:ASP:O	3:F:402:HOH:O	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:HIS:CG	1:F:203:ARG:NH1	2.48	0.81
1:B:57:LEU:O	3:B:402:HOH:O	1.99	0.80
1:E:97:VAL:HG13	2:E:301:NDP:H2A	1.64	0.79
1:G:42:GLU:HA	1:G:65:ARG:NH1	1.98	0.79
1:A:133:LEU:O	3:A:401:HOH:O	2.01	0.78
1:E:43:GLU:H	1:E:65:ARG:NH2	1.84	0.75
1:E:16:GLY:HA2	2:E:301:NDP:H1B	1.67	0.75
1:C:59:GLY:N	3:C:401:HOH:O	2.12	0.75
1:F:43:GLU:H	1:F:65:ARG:HH21	1.35	0.75
1:F:199:PRO:HD2	1:F:202:GLU:OE2	1.87	0.74
1:E:43:GLU:HG2	1:E:65:ARG:NH2	2.04	0.73
1:G:151:ILE:HB	1:G:154:ARG:HH12	1.54	0.73
1:D:200:ASP:N	1:D:202:GLU:OE2	2.22	0.72
1:C:151:ILE:CG2	1:C:154:ARG:NH1	2.52	0.72
1:H:49:SER:O	1:H:53:GLU:HG3	1.90	0.71
1:B:112:GLN:NE2	3:B:403:HOH:O	2.15	0.71
1:F:203:ARG:HA	1:F:204:ALA:HB2	1.72	0.71
1:C:151:ILE:HG21	1:C:154:ARG:HH12	1.56	0.70
1:F:114:ILE:HG12	1:F:156:HIS:HD2	1.57	0.70
1:G:41:ARG:NH2	1:G:42:GLU:OE1	2.25	0.69
1:A:200:ASP:OD1	1:A:203:ARG:NH2	2.26	0.69
1:G:151:ILE:HB	1:G:154:ARG:HH11	1.57	0.68
1:H:188:GLY:O	2:H:301:NDP:H42N	1.93	0.68
1:E:163:ALA:HB2	1:H:163:ALA:HB2	1.76	0.68
1:B:83:ARG:NH2	3:B:407:HOH:O	2.27	0.68
1:D:204:ALA:O	1:D:208:LYS:HE2	1.93	0.68
1:E:60:ASP:OD2	3:E:401:HOH:O	2.11	0.67
1:H:43:GLU:OE2	3:H:402:HOH:O	2.11	0.67
1:B:163:ALA:HB2	1:C:163:ALA:HB2	1.76	0.67
1:F:196:HIS:CG	1:F:203:ARG:HH11	2.14	0.66
1:E:97:VAL:CG1	2:E:301:NDP:H2A	2.26	0.66
1:F:196:HIS:CD2	1:F:203:ARG:HH12	2.14	0.66
1:F:49:SER:O	1:F:53:GLU:HB2	1.96	0.66
1:E:72:LYS:O	1:E:76:GLU:HG3	1.96	0.65
1:G:5:LEU:N	3:G:401:HOH:O	2.27	0.65
1:H:191:GLU:OE2	3:H:403:HOH:O	2.14	0.65
1:H:72:LYS:O	1:H:76:GLU:HG3	1.96	0.65
1:C:161:LYS:NZ	3:C:402:HOH:O	2.25	0.64
1:G:43:GLU:N	1:G:65:ARG:HH22	1.94	0.64
1:A:163:ALA:HB2	1:D:163:ALA:HB2	1.79	0.64
1:D:11:LYS:HE3	1:D:85:PHE:CD1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:VAL:CG1	2:F:301:NDP:H2A	2.28	0.64
1:B:195:LEU:HD22	1:B:198:LEU:HD12	1.80	0.63
1:E:43:GLU:HG2	1:E:65:ARG:HH22	1.61	0.63
1:F:144:SER:OG	2:F:301:NDP:H5N	1.99	0.63
1:B:151:ILE:HG13	1:B:154:ARG:HB2	1.81	0.62
1:C:53:GLU:O	1:C:57:LEU:HD23	1.99	0.62
1:F:200:ASP:HA	1:F:203:ARG:H	1.65	0.62
1:B:53:GLU:CD	3:B:401:HOH:O	2.34	0.62
1:F:68:LEU:H	2:F:301:NDP:H61A	1.47	0.61
1:E:4:GLU:CD	1:E:5:LEU:H	2.04	0.61
1:F:98:ILE:HD11	1:F:154:ARG:HE	1.66	0.61
1:F:112:GLN:NE2	3:F:401:HOH:O	1.87	0.61
1:B:53:GLU:CG	3:B:401:HOH:O	2.39	0.60
1:D:100:HIS:CD2	1:D:154:ARG:HD3	2.36	0.60
1:F:114:ILE:HG12	1:F:156:HIS:CD2	2.36	0.60
1:A:245:ILE:HD12	1:H:245:ILE:HG23	1.85	0.59
1:C:199:PRO:HD2	1:C:202:GLU:OE2	2.01	0.59
1:C:201:ASP:HB3	1:C:204:ALA:HB3	1.84	0.59
1:F:188:GLY:O	2:F:301:NDP:H42N	2.03	0.59
1:C:245:ILE:HD12	1:F:245:ILE:HG23	1.85	0.58
1:G:163:ALA:HB2	1:F:163:ALA:HB2	1.85	0.58
1:A:198:LEU:O	1:A:203:ARG:NH1	2.37	0.58
1:F:185:LEU:HD23	1:F:245:ILE:HB	1.86	0.58
1:D:208:LYS:O	1:D:212:THR:HG23	2.04	0.58
1:E:185:LEU:HD23	1:E:245:ILE:HB	1.86	0.57
1:H:251:ILE:O	1:H:252:SER:OG	2.21	0.57
1:C:5:LEU:HB3	1:C:7:LEU:HG	1.85	0.57
1:F:204:ALA:HB3	1:F:207:THR:HB	1.87	0.56
1:G:185:LEU:HD23	1:G:245:ILE:HB	1.87	0.56
1:F:196:HIS:CG	1:F:203:ARG:HH12	2.23	0.56
1:E:43:GLU:HG2	1:E:65:ARG:CZ	2.35	0.56
1:F:37:PHE:CZ	1:F:64:LEU:HD23	2.41	0.56
1:H:133:LEU:O	3:H:404:HOH:O	2.18	0.56
1:F:203:ARG:HA	1:F:204:ALA:CB	2.34	0.56
1:F:43:GLU:H	1:F:65:ARG:NH2	2.03	0.56
1:B:31:ARG:NH1	3:B:404:HOH:O	2.28	0.56
1:C:201:ASP:HA	1:C:204:ALA:N	2.16	0.55
1:C:100:HIS:CE1	1:C:154:ARG:HE	2.24	0.55
1:H:223:ASP:OD1	3:H:405:HOH:O	2.18	0.55
1:F:196:HIS:CD2	1:F:203:ARG:NH1	2.74	0.55
1:D:112:GLN:NE2	3:D:406:HOH:O	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:HG2	1:B:202:GLU:O	2.07	0.55
1:F:207:THR:O	1:F:211:SER:HB2	2.06	0.55
1:G:40:TYR:HE2	1:G:65:ARG:NH2	2.05	0.54
1:G:43:GLU:HG2	1:G:65:ARG:NH2	2.21	0.54
1:D:4:GLU:HG2	1:D:5:LEU:N	2.22	0.54
1:E:188:GLY:O	2:E:301:NDP:H42N	2.07	0.54
1:C:100:HIS:CE1	1:C:154:ARG:HH21	2.25	0.54
1:E:145:LYS:HE3	3:E:410:HOH:O	2.06	0.53
1:G:5:LEU:HD23	1:G:236:LEU:HD12	1.89	0.53
1:B:190:VAL:H	2:B:301:NDP:H72N	1.54	0.53
1:H:93:ASN:ND2	3:H:406:HOH:O	2.27	0.53
1:G:145:LYS:HE3	3:G:420:HOH:O	2.09	0.53
1:F:46:ALA:HA	3:F:402:HOH:O	2.08	0.53
1:F:42:GLU:HA	1:F:65:ARG:HH21	1.74	0.53
1:B:53:GLU:CB	3:B:401:HOH:O	2.08	0.52
1:C:5:LEU:HD22	1:F:3:LEU:O	2.09	0.52
1:E:43:GLU:HG2	1:E:65:ARG:NH1	2.23	0.52
1:B:58:GLY:CA	3:B:402:HOH:O	2.50	0.52
1:B:188:GLY:O	2:B:301:NDP:H42N	2.10	0.52
1:C:11:LYS:HD3	1:C:85:PHE:CG	2.45	0.52
1:G:188:GLY:O	2:G:301:NDP:H42N	2.10	0.52
1:D:201:ASP:N	1:D:202:GLU:OE2	2.43	0.52
1:C:190:VAL:H	2:C:301:NDP:H72N	1.58	0.51
1:F:97:VAL:HG13	2:F:301:NDP:H2A	1.92	0.51
1:B:155:ALA:HB1	1:C:167:LEU:HD12	1.93	0.51
1:C:80:GLU:HG3	1:C:84:ARG:HE	1.76	0.51
1:E:126:ILE:O	1:E:130:ILE:HG12	2.10	0.51
1:G:245:ILE:HD12	1:B:245:ILE:HG23	1.92	0.51
1:G:40:TYR:CE2	1:G:65:ARG:NH2	2.79	0.51
1:F:100:HIS:NE2	1:F:154:ARG:NH1	2.59	0.50
1:A:112:GLN:NE2	3:A:402:HOH:O	2.11	0.50
1:C:185:LEU:HD23	1:C:245:ILE:HB	1.92	0.50
1:D:188:GLY:O	2:D:301:NDP:H42N	2.12	0.50
1:D:198:LEU:HB3	1:D:202:GLU:CG	2.42	0.50
1:C:214:THR:HA	1:C:251:ILE:HA	1.94	0.50
1:E:5:LEU:O	1:E:234:SER:HB2	2.12	0.50
1:G:5:LEU:O	1:G:234:SER:HB2	2.11	0.49
1:D:145:LYS:HE3	3:D:416:HOH:O	2.11	0.49
1:E:199:PRO:O	1:E:201:ASP:N	2.45	0.49
1:E:26:VAL:HG13	1:E:36:VAL:HG11	1.93	0.49
1:B:126:ILE:O	1:B:130:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:HIS:CD2	1:G:154:ARG:HE	2.31	0.48
1:A:188:GLY:O	2:A:301:NDP:H42N	2.13	0.48
1:E:42:GLU:OE2	1:E:65:ARG:NH2	2.45	0.48
1:D:56:GLN:NE2	3:D:405:HOH:O	2.30	0.48
1:H:38:THR:HG21	1:H:50:LEU:HD21	1.96	0.48
1:F:43:GLU:N	1:F:65:ARG:HH21	2.06	0.47
1:C:198:LEU:HB3	1:C:199:PRO:HD2	1.96	0.47
1:E:214:THR:HA	1:E:251:ILE:HA	1.97	0.47
1:G:151:ILE:HD12	1:G:154:ARG:HD2	1.97	0.47
1:G:43:GLU:N	1:G:65:ARG:NH2	2.61	0.47
1:C:188:GLY:O	2:C:301:NDP:H42N	2.15	0.47
1:H:5:LEU:O	1:H:234:SER:HB2	2.15	0.47
1:E:199:PRO:HG2	1:E:202:GLU:OE1	2.15	0.47
1:A:252:SER:O	1:E:149:VAL:HG13	2.15	0.47
1:F:68:LEU:N	2:F:301:NDP:H61A	2.13	0.47
1:A:200:ASP:HA	1:A:203:ARG:HB3	1.98	0.46
2:F:301:NDP:N3A	2:F:301:NDP:H2B	2.30	0.46
1:A:151:ILE:CG2	1:A:154:ARG:NH1	2.78	0.46
1:G:52:ARG:HA	1:G:55:LYS:HE3	1.96	0.46
1:D:5:LEU:O	1:D:234:SER:HB2	2.15	0.45
1:F:171:LEU:HD23	1:F:182:PHE:CE2	2.51	0.45
1:F:207:THR:O	1:F:211:SER:CB	2.63	0.45
1:C:80:GLU:O	1:C:84:ARG:HG3	2.15	0.45
1:D:214:THR:HA	1:D:251:ILE:HA	1.99	0.45
1:G:199:PRO:HG2	1:G:202:GLU:OE2	2.17	0.45
1:F:52:ARG:HB2	1:F:52:ARG:NH1	2.32	0.45
2:E:301:NDP:H2B	2:E:301:NDP:N3A	2.32	0.45
1:B:214:THR:HA	1:B:251:ILE:HA	1.98	0.45
1:B:185:LEU:HD23	1:B:245:ILE:HB	1.99	0.45
1:F:42:GLU:CA	1:F:65:ARG:HH21	2.29	0.45
1:G:190:VAL:H	2:G:301:NDP:H72N	1.64	0.45
1:D:194:GLU:O	1:D:194:GLU:HG3	2.17	0.45
1:H:4:GLU:CD	1:H:4:GLU:H	2.20	0.45
1:E:3:LEU:O	3:E:402:HOH:O	2.21	0.44
1:H:199:PRO:C	1:H:201:ASP:H	2.20	0.44
1:H:15:THR:O	1:H:94:ASN:HB3	2.17	0.44
1:C:202:GLU:O	1:C:206:MET:HG2	2.18	0.44
1:A:151:ILE:HG22	1:A:154:ARG:HH12	1.83	0.44
1:C:13:LEU:HD12	1:C:37:PHE:O	2.17	0.44
1:H:161:LYS:HA	1:H:161:LYS:HD2	1.77	0.44
1:D:191:GLU:OE1	1:D:196:HIS:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLY:CA	3:C:401:HOH:O	2.51	0.43
1:D:100:HIS:CD2	1:D:154:ARG:CD	3.01	0.43
1:C:13:LEU:HA	1:C:37:PHE:O	2.18	0.43
1:E:4:GLU:CD	1:E:5:LEU:N	2.72	0.43
1:F:114:ILE:HD11	1:F:156:HIS:HB2	2.00	0.43
1:C:80:GLU:HG3	1:C:84:ARG:NE	2.32	0.43
1:F:126:ILE:O	1:F:130:ILE:HG13	2.18	0.43
1:H:145:LYS:NZ	1:H:252:SER:OG	2.52	0.43
1:C:4:GLU:HG2	1:C:5:LEU:N	2.33	0.43
1:F:200:ASP:CA	1:F:203:ARG:H	2.30	0.43
1:A:185:LEU:HD23	1:A:245:ILE:HB	2.00	0.43
1:C:161:LYS:HA	1:C:161:LYS:HD2	1.83	0.43
1:B:97:VAL:HG23	1:B:114:ILE:HG13	2.01	0.42
1:H:185:LEU:HD23	1:H:245:ILE:HB	2.01	0.42
1:D:5:LEU:HD23	1:D:236:LEU:HD12	2.00	0.42
1:E:245:ILE:HG23	1:D:245:ILE:HD12	2.01	0.42
1:F:114:ILE:HD12	1:F:160:THR:HG21	2.01	0.42
1:B:161:LYS:HA	1:B:161:LYS:HD2	1.85	0.42
1:E:128:HIS:O	1:E:131:PRO:HD2	2.19	0.42
1:H:214:THR:HA	1:H:251:ILE:HA	2.02	0.42
1:G:98:ILE:HD11	1:G:154:ARG:HD3	2.00	0.42
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.89	0.42
1:D:151:ILE:CG2	1:D:154:ARG:CZ	2.97	0.42
1:D:198:LEU:HA	1:D:199:PRO:HD3	1.94	0.42
1:H:151:ILE:HG21	1:H:154:ARG:CZ	2.50	0.42
1:E:15:THR:O	1:E:94:ASN:HB3	2.20	0.42
1:H:21:VAL:HB	2:H:301:NDP:H51N	2.01	0.42
1:G:113:ARG:NH1	3:G:402:HOH:O	2.29	0.41
1:G:55:LYS:HD2	1:G:56:GLN:N	2.35	0.41
1:G:41:ARG:C	1:G:65:ARG:NH1	2.70	0.41
1:F:15:THR:O	1:F:94:ASN:HB3	2.20	0.41
1:B:196:HIS:CE1	1:B:203:ARG:NH1	2.88	0.41
1:B:199:PRO:O	1:B:203:ARG:HB2	2.21	0.41
1:C:3:LEU:O	1:F:5:LEU:HD12	2.21	0.41
1:B:100:HIS:HB3	1:B:153:LEU:HD23	2.02	0.41
1:E:16:GLY:CA	2:E:301:NDP:H1B	2.45	0.41
1:F:202:GLU:C	1:F:204:ALA:HA	2.40	0.41
1:C:195:LEU:HA	1:C:198:LEU:HD12	2.03	0.41
1:C:208:LYS:HA	1:C:208:LYS:HD2	1.90	0.41
1:D:185:LEU:HD23	1:D:245:ILE:HB	2.02	0.41
1:A:214:THR:HA	1:A:251:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:VAL:HG23	1:C:114:ILE:HG13	2.03	0.41
1:B:198:LEU:HD13	1:B:202:GLU:O	2.21	0.41
1:D:151:ILE:HG21	1:D:154:ARG:CZ	2.51	0.41
1:B:39:CYS:HA	1:B:64:LEU:O	2.21	0.41
1:G:167:LEU:HD12	1:F:155:ALA:HB1	2.02	0.41
1:E:39:CYS:HA	1:E:64:LEU:O	2.20	0.40
1:F:16:GLY:CA	2:F:301:NDP:H1B	2.40	0.40
1:C:157:TYR:O	1:C:161:LYS:HG2	2.21	0.40
1:G:214:THR:HA	1:G:251:ILE:HA	2.02	0.40
1:F:51:ALA:O	1:F:55:LYS:HG3	2.21	0.40
1:B:210:TYR:O	1:B:213:LYS:HB2	2.22	0.40
1:C:100:HIS:N	1:C:100:HIS:CD2	2.89	0.40
1:E:151:ILE:HG21	1:E:154:ARG:CZ	2.52	0.40

All (1) 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:E:45:ASP:OD2	1:H:83:ARG:NH1[2_554]	2.14	0.06

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	246/272 (90%)	239 (97%)	6 (2%)	1 (0%)	39 48
1	B	248/272 (91%)	241 (97%)	7 (3%)	0	100 100
1	C	248/272 (91%)	244 (98%)	4 (2%)	0	100 100
1	D	248/272 (91%)	240 (97%)	8 (3%)	0	100 100
1	E	248/272 (91%)	243 (98%)	4 (2%)	1 (0%)	39 48
1	F	248/272 (91%)	241 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	246/272 (90%)	242 (98%)	3 (1%)	1 (0%)	39 48
1	H	248/272 (91%)	242 (98%)	6 (2%)	0	100 100
All	All	1980/2176 (91%)	1932 (98%)	45 (2%)	3 (0%)	52 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	200	ASP
1	A	200	ASP
1	G	200	ASP

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	191/212 (90%)	191 (100%)	0	100 100
1	B	193/212 (91%)	192 (100%)	1 (0%)	92 97
1	C	193/212 (91%)	191 (99%)	2 (1%)	82 91
1	D	193/212 (91%)	191 (99%)	2 (1%)	82 91
1	E	193/212 (91%)	191 (99%)	2 (1%)	82 91
1	F	193/212 (91%)	191 (99%)	2 (1%)	82 91
1	G	191/212 (90%)	188 (98%)	3 (2%)	70 84
1	H	193/212 (91%)	188 (97%)	5 (3%)	54 71
All	All	1540/1696 (91%)	1523 (99%)	17 (1%)	80 90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	55	LYS
1	G	200	ASP
1	G	201	ASP
1	B	203	ARG

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Mol	Chain	Res	Type
1	C	56	GLN
1	C	154	ARG
1	F	3	LEU
1	F	196	HIS
1	E	201	ASP
1	E	206	MET
1	H	45	ASP
1	H	145	LYS
1	H	154	ARG
1	H	180	LEU
1	H	203	ARG
1	D	202	GLU
1	D	208	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	HIS
1	C	100	HIS
1	A	79	GLN
1	D	100	HIS

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	NDP	A	301	-	44,52,52	3.97	21 (47%)	55,80,80	2.52	6 (10%)
2	NDP	B	301	-	44,52,52	4.10	20 (45%)	55,80,80	2.56	7 (12%)
2	NDP	C	301	-	44,52,52	4.05	19 (43%)	55,80,80	2.68	8 (14%)
2	NDP	D	301	-	44,52,52	4.18	19 (43%)	55,80,80	2.60	4 (7%)
2	NDP	E	301	-	44,52,52	4.06	16 (36%)	55,80,80	3.06	8 (14%)
2	NDP	F	301	-	44,52,52	4.14	16 (36%)	55,80,80	2.89	7 (12%)
2	NDP	G	301	-	44,52,52	4.11	19 (43%)	55,80,80	2.53	5 (9%)
2	NDP	H	301	-	44,52,52	3.97	19 (43%)	55,80,80	2.67	8 (14%)

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	NDP	A	301	-	-	0/30/77/77	0/5/5/5
2	NDP	B	301	-	-	0/30/77/77	0/5/5/5
2	NDP	C	301	-	-	0/30/77/77	0/5/5/5
2	NDP	D	301	-	-	0/30/77/77	0/5/5/5
2	NDP	E	301	-	-	0/30/77/77	0/5/5/5
2	NDP	F	301	-	-	0/30/77/77	0/5/5/5
2	NDP	G	301	-	-	0/30/77/77	0/5/5/5
2	NDP	H	301	-	-	0/30/77/77	0/5/5/5

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NDP	C2B-C1B	-8.17	1.30	1.53
2	G	301	NDP	C2B-C1B	-7.87	1.31	1.53
2	D	301	NDP	C2B-C1B	-7.85	1.31	1.53
2	F	301	NDP	C2B-C1B	-7.74	1.32	1.53
2	H	301	NDP	C2B-C1B	-7.57	1.32	1.53
2	E	301	NDP	C2B-C1B	-7.45	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NDP	C2B-C1B	-7.31	1.33	1.53
2	A	301	NDP	C2B-C1B	-7.27	1.33	1.53
2	H	301	NDP	C2D-C1D	-7.17	1.30	1.53
2	F	301	NDP	C2D-C1D	-7.04	1.31	1.53
2	D	301	NDP	C2D-C1D	-7.03	1.31	1.53
2	B	301	NDP	C2D-C1D	-7.03	1.31	1.53
2	A	301	NDP	C2D-C1D	-6.86	1.31	1.53
2	E	301	NDP	C2D-C1D	-6.71	1.32	1.53
2	G	301	NDP	C2D-C1D	-6.62	1.32	1.53
2	C	301	NDP	C2D-C1D	-6.51	1.32	1.53
2	G	301	NDP	O4B-C4B	-6.20	1.30	1.45
2	F	301	NDP	O4D-C4D	-6.03	1.31	1.45
2	E	301	NDP	O4D-C4D	-6.02	1.31	1.45
2	H	301	NDP	O4D-C4D	-5.86	1.31	1.45
2	D	301	NDP	O4B-C4B	-5.86	1.31	1.45
2	C	301	NDP	O4B-C4B	-5.73	1.31	1.45
2	D	301	NDP	O4D-C4D	-5.68	1.32	1.45
2	B	301	NDP	O4D-C4D	-5.67	1.32	1.45
2	B	301	NDP	O4B-C4B	-5.65	1.32	1.45
2	C	301	NDP	O4D-C4D	-5.60	1.32	1.45
2	A	301	NDP	O4B-C4B	-5.40	1.32	1.45
2	H	301	NDP	O4B-C4B	-5.38	1.32	1.45
2	G	301	NDP	O4D-C4D	-5.38	1.32	1.45
2	F	301	NDP	O4B-C4B	-5.25	1.33	1.45
2	A	301	NDP	O4D-C4D	-5.18	1.33	1.45
2	E	301	NDP	O4B-C4B	-4.76	1.34	1.45
2	D	301	NDP	C5A-C4A	-3.17	1.33	1.40
2	H	301	NDP	C5A-C4A	-3.07	1.33	1.40
2	F	301	NDP	O3B-C3B	-2.99	1.35	1.43
2	C	301	NDP	O3D-C3D	-2.96	1.36	1.43
2	A	301	NDP	O3B-C3B	-2.96	1.36	1.43
2	D	301	NDP	O3D-C3D	-2.92	1.36	1.43
2	B	301	NDP	O3D-C3D	-2.92	1.36	1.43
2	G	301	NDP	O3D-C3D	-2.89	1.36	1.43
2	E	301	NDP	O3D-C3D	-2.81	1.36	1.43
2	G	301	NDP	C5A-C4A	-2.75	1.34	1.40
2	C	301	NDP	C5A-C4A	-2.71	1.34	1.40
2	B	301	NDP	O3B-C3B	-2.71	1.36	1.43
2	C	301	NDP	O3B-C3B	-2.59	1.36	1.43
2	A	301	NDP	C5A-C4A	-2.56	1.34	1.40
2	B	301	NDP	C5A-C4A	-2.51	1.34	1.40
2	F	301	NDP	O3D-C3D	-2.45	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NDP	O3B-C3B	-2.39	1.37	1.43
2	H	301	NDP	O3B-C3B	-2.35	1.37	1.43
2	A	301	NDP	O3D-C3D	-2.34	1.37	1.43
2	H	301	NDP	O7N-C7N	-2.33	1.18	1.24
2	G	301	NDP	O7N-C7N	-2.33	1.18	1.24
2	A	301	NDP	O7N-C7N	-2.26	1.18	1.24
2	C	301	NDP	O7N-C7N	-2.24	1.18	1.24
2	E	301	NDP	O3B-C3B	-2.24	1.37	1.43
2	G	301	NDP	O3B-C3B	-2.22	1.37	1.43
2	H	301	NDP	O3D-C3D	-2.13	1.37	1.43
2	B	301	NDP	O7N-C7N	-2.06	1.19	1.24
2	A	301	NDP	O2B-C2B	2.05	1.50	1.44
2	B	301	NDP	C2N-N1N	2.08	1.41	1.37
2	A	301	NDP	C2A-N1A	2.08	1.37	1.33
2	D	301	NDP	C2A-N3A	2.09	1.35	1.32
2	G	301	NDP	C2A-N3A	2.09	1.35	1.32
2	H	301	NDP	C2N-N1N	2.11	1.41	1.37
2	D	301	NDP	O2B-C2B	2.15	1.50	1.44
2	B	301	NDP	C2A-N1A	2.17	1.38	1.33
2	H	301	NDP	C2A-N3A	2.21	1.36	1.32
2	B	301	NDP	C2A-N3A	2.25	1.36	1.32
2	G	301	NDP	O2D-C2D	2.38	1.48	1.43
2	C	301	NDP	C6N-N1N	2.42	1.43	1.37
2	E	301	NDP	C6A-N6A	2.45	1.44	1.34
2	D	301	NDP	C6A-N6A	2.48	1.44	1.34
2	F	301	NDP	C6N-N1N	2.50	1.43	1.37
2	G	301	NDP	C6N-N1N	2.54	1.43	1.37
2	C	301	NDP	C2A-N3A	2.55	1.36	1.32
2	A	301	NDP	C6N-N1N	2.60	1.44	1.37
2	A	301	NDP	C6A-N6A	2.61	1.44	1.34
2	H	301	NDP	C6A-N6A	2.61	1.44	1.34
2	A	301	NDP	C2A-N3A	2.68	1.36	1.32
2	C	301	NDP	C6A-N6A	2.70	1.45	1.34
2	G	301	NDP	C2N-N1N	2.71	1.42	1.37
2	C	301	NDP	C2N-N1N	2.72	1.42	1.37
2	F	301	NDP	C6A-N6A	2.73	1.45	1.34
2	G	301	NDP	C6A-N6A	2.78	1.45	1.34
2	E	301	NDP	C2N-N1N	2.82	1.42	1.37
2	D	301	NDP	O2D-C2D	2.83	1.49	1.43
2	B	301	NDP	C6A-N6A	2.85	1.45	1.34
2	F	301	NDP	C2N-N1N	2.85	1.42	1.37
2	B	301	NDP	O2D-C2D	2.87	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NDP	C6N-N1N	2.88	1.44	1.37
2	H	301	NDP	O2D-C2D	2.92	1.49	1.43
2	A	301	NDP	C2N-N1N	2.93	1.42	1.37
2	E	301	NDP	C6N-N1N	2.96	1.45	1.37
2	B	301	NDP	C6N-N1N	2.99	1.45	1.37
2	H	301	NDP	C6N-N1N	3.01	1.45	1.37
2	F	301	NDP	O2D-C2D	3.03	1.50	1.43
2	E	301	NDP	O2D-C2D	3.13	1.50	1.43
2	A	301	NDP	O2D-C2D	3.24	1.50	1.43
2	E	301	NDP	C4N-C5N	3.33	1.56	1.49
2	C	301	NDP	C4N-C5N	3.36	1.56	1.49
2	C	301	NDP	O2D-C2D	3.40	1.51	1.43
2	B	301	NDP	C4N-C5N	3.41	1.56	1.49
2	D	301	NDP	C2N-N1N	3.45	1.43	1.37
2	H	301	NDP	C4N-C5N	3.52	1.56	1.49
2	A	301	NDP	C4N-C5N	3.60	1.56	1.49
2	G	301	NDP	C4N-C5N	3.63	1.56	1.49
2	D	301	NDP	C4N-C5N	3.70	1.56	1.49
2	F	301	NDP	C4N-C5N	3.72	1.57	1.49
2	H	301	NDP	C7N-N7N	4.04	1.45	1.33
2	A	301	NDP	C7N-N7N	4.06	1.45	1.33
2	E	301	NDP	C7N-N7N	4.10	1.45	1.33
2	B	301	NDP	C7N-N7N	4.11	1.45	1.33
2	G	301	NDP	C7N-N7N	4.13	1.45	1.33
2	C	301	NDP	C7N-N7N	4.16	1.45	1.33
2	D	301	NDP	C7N-N7N	4.20	1.45	1.33
2	F	301	NDP	C7N-N7N	4.40	1.46	1.33
2	B	301	NDP	C2N-C3N	5.65	1.50	1.34
2	H	301	NDP	C2N-C3N	5.79	1.50	1.34
2	A	301	NDP	C2N-C3N	5.85	1.51	1.34
2	G	301	NDP	C2N-C3N	5.88	1.51	1.34
2	C	301	NDP	C2N-C3N	5.92	1.51	1.34
2	E	301	NDP	C2N-C3N	5.98	1.51	1.34
2	F	301	NDP	C2N-C3N	6.08	1.51	1.34
2	D	301	NDP	C2N-C3N	6.18	1.51	1.34
2	A	301	NDP	O4D-C1D	7.41	1.60	1.42
2	E	301	NDP	O4D-C1D	7.49	1.60	1.42
2	F	301	NDP	O4D-C1D	7.57	1.60	1.42
2	C	301	NDP	O4D-C1D	7.65	1.60	1.42
2	H	301	NDP	O4D-C1D	7.69	1.61	1.42
2	G	301	NDP	O4D-C1D	7.74	1.61	1.42
2	B	301	NDP	O4D-C1D	7.75	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NDP	O4D-C1D	8.13	1.62	1.42
2	H	301	NDP	C6N-C5N	11.62	1.54	1.33
2	C	301	NDP	C6N-C5N	11.84	1.55	1.33
2	B	301	NDP	C6N-C5N	11.91	1.55	1.33
2	F	301	NDP	C6N-C5N	12.01	1.55	1.33
2	E	301	NDP	C6N-C5N	12.02	1.55	1.33
2	D	301	NDP	C6N-C5N	12.15	1.55	1.33
2	G	301	NDP	C6N-C5N	12.15	1.55	1.33
2	A	301	NDP	C6N-C5N	12.63	1.56	1.33
2	A	301	NDP	O4B-C1B	12.89	1.59	1.41
2	H	301	NDP	O4B-C1B	13.34	1.60	1.41
2	C	301	NDP	O4B-C1B	13.94	1.61	1.41
2	G	301	NDP	O4B-C1B	14.63	1.62	1.41
2	E	301	NDP	O4B-C1B	14.71	1.62	1.41
2	D	301	NDP	O4B-C1B	14.73	1.62	1.41
2	B	301	NDP	O4B-C1B	14.86	1.62	1.41
2	F	301	NDP	O4B-C1B	15.08	1.62	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	NDP	C1B-N9A-C4A	-12.64	112.69	126.81
2	D	301	NDP	C1B-N9A-C4A	-12.29	113.09	126.81
2	F	301	NDP	C1B-N9A-C4A	-12.20	113.20	126.81
2	A	301	NDP	C1B-N9A-C4A	-12.09	113.32	126.81
2	E	301	NDP	C1B-N9A-C4A	-12.04	113.36	126.81
2	C	301	NDP	C1B-N9A-C4A	-11.82	113.62	126.81
2	G	301	NDP	C1B-N9A-C4A	-11.73	113.72	126.81
2	B	301	NDP	C1B-N9A-C4A	-11.50	113.97	126.81
2	B	301	NDP	N3A-C2A-N1A	-11.45	119.88	128.87
2	H	301	NDP	N3A-C2A-N1A	-11.25	120.03	128.87
2	C	301	NDP	N3A-C2A-N1A	-11.08	120.17	128.87
2	E	301	NDP	N3A-C2A-N1A	-10.84	120.35	128.87
2	G	301	NDP	N3A-C2A-N1A	-10.70	120.47	128.87
2	D	301	NDP	N3A-C2A-N1A	-10.63	120.52	128.87
2	A	301	NDP	N3A-C2A-N1A	-10.44	120.67	128.87
2	F	301	NDP	N3A-C2A-N1A	-9.73	121.23	128.87
2	E	301	NDP	N6A-C6A-N1A	-9.11	103.23	118.52
2	F	301	NDP	N6A-C6A-N1A	-8.82	103.72	118.52
2	D	301	NDP	N6A-C6A-N1A	-7.92	105.22	118.52
2	C	301	NDP	N6A-C6A-N1A	-7.63	105.72	118.52
2	G	301	NDP	N6A-C6A-N1A	-7.28	106.30	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	NDP	C4B-O4B-C1B	-6.82	102.42	109.64
2	H	301	NDP	N6A-C6A-N1A	-6.75	107.19	118.52
2	A	301	NDP	N6A-C6A-N1A	-6.34	107.88	118.52
2	B	301	NDP	N6A-C6A-N1A	-6.27	108.00	118.52
2	E	301	NDP	C4B-O4B-C1B	-6.24	103.03	109.64
2	E	301	NDP	O4B-C1B-C2B	-5.17	97.31	106.60
2	F	301	NDP	O4B-C1B-C2B	-4.34	98.79	106.60
2	C	301	NDP	C4B-O4B-C1B	-4.00	105.41	109.64
2	B	301	NDP	C4N-C5N-C6N	-3.13	117.41	122.58
2	D	301	NDP	C2B-C1B-N9A	-2.89	105.22	113.48
2	H	301	NDP	C4N-C5N-C6N	-2.83	117.92	122.58
2	B	301	NDP	C2B-C1B-N9A	-2.81	105.44	113.48
2	H	301	NDP	C3N-C2N-N1N	-2.75	119.20	123.24
2	E	301	NDP	C3N-C2N-N1N	-2.67	119.31	123.24
2	A	301	NDP	C2B-C1B-N9A	-2.60	106.06	113.48
2	E	301	NDP	C4N-C5N-C6N	-2.55	118.37	122.58
2	H	301	NDP	C4B-O4B-C1B	-2.47	107.03	109.64
2	F	301	NDP	C3N-C2N-N1N	-2.45	119.64	123.24
2	H	301	NDP	C2B-C1B-N9A	-2.25	107.03	113.48
2	G	301	NDP	C4N-C5N-C6N	-2.20	118.95	122.58
2	B	301	NDP	C4B-O4B-C1B	-2.10	107.42	109.64
2	G	301	NDP	C4B-O4B-C1B	-2.09	107.43	109.64
2	A	301	NDP	C4N-C5N-C6N	-2.08	119.14	122.58
2	C	301	NDP	O5D-C5D-C4D	-2.06	101.66	109.09
2	C	301	NDP	C2B-C1B-N9A	-2.06	107.59	113.48
2	B	301	NDP	O2X-P2B-O2B	2.08	112.83	106.62
2	H	301	NDP	O3X-P2B-O2B	2.27	113.41	106.62
2	C	301	NDP	O4B-C1B-N9A	2.35	112.55	108.11
2	A	301	NDP	O2X-P2B-O2B	2.79	114.98	106.62
2	C	301	NDP	O2B-P2B-O1X	2.94	114.50	107.48
2	F	301	NDP	O4B-C1B-N9A	6.23	119.87	108.11
2	E	301	NDP	O4B-C1B-N9A	7.36	122.02	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NDP	1	0
2	B	301	NDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NDP	2	0
2	D	301	NDP	1	0
2	E	301	NDP	6	0
2	F	301	NDP	9	0
2	G	301	NDP	2	0
2	H	301	NDP	3	0

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	248/272 (91%)	-0.23	2 (0%)	87 90	20, 29, 51, 78	0
1	B	250/272 (91%)	-0.15	4 (1%)	74 80	21, 32, 61, 94	0
1	C	250/272 (91%)	0.07	8 (3%)	51 60	24, 38, 69, 92	0
1	D	250/272 (91%)	-0.21	2 (0%)	87 90	19, 29, 55, 86	0
1	E	250/272 (91%)	-0.13	6 (2%)	62 71	19, 29, 59, 94	0
1	F	250/272 (91%)	0.02	8 (3%)	51 60	22, 36, 70, 101	0
1	G	248/272 (91%)	-0.17	4 (1%)	74 80	21, 33, 56, 89	0
1	H	250/272 (91%)	-0.18	3 (1%)	81 85	19, 28, 55, 89	0
All	All	1996/2176 (91%)	-0.12	37 (1%)	70 76	19, 31, 63, 101	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	SER	5.9
1	F	198	LEU	4.6
1	F	201	ASP	4.6
1	H	252	SER	4.0
1	D	199	PRO	3.9
1	F	197	ALA	3.7
1	E	200	ASP	3.4
1	C	82	GLY	3.3
1	F	199	PRO	3.3
1	A	135	ASP	3.2
1	B	252	SER	3.1
1	F	195	LEU	3.1
1	B	202	GLU	3.1
1	C	197	ALA	3.1
1	G	42	GLU	2.9
1	C	58	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	196	HIS	2.7
1	C	64	LEU	2.7
1	G	202	GLU	2.7
1	C	200	ASP	2.7
1	C	135	ASP	2.6
1	H	194	GLU	2.6
1	E	194	GLU	2.6
1	B	58	GLY	2.6
1	F	194	GLU	2.5
1	E	45	ASP	2.5
1	H	201	ASP	2.5
1	E	58	GLY	2.4
1	F	205	GLU	2.3
1	G	200	ASP	2.3
1	F	252	SER	2.3
1	C	55	LYS	2.2
1	B	200	ASP	2.2
1	A	201	ASP	2.2
1	G	201	ASP	2.2
1	D	252	SER	2.2
1	E	197	ALA	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
2	NDP	F	301	48/48	0.90	0.21	1.14	39,48,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NDP	D	301	48/48	0.95	0.14	0.59	29,38,43,45	0
2	NDP	C	301	48/48	0.95	0.16	0.29	33,48,57,63	0
2	NDP	A	301	48/48	0.97	0.12	0.03	26,31,37,39	0
2	NDP	B	301	48/48	0.95	0.13	0.02	31,38,48,49	0
2	NDP	E	301	48/48	0.94	0.13	-0.09	24,36,43,47	0
2	NDP	H	301	48/48	0.97	0.13	-0.10	27,33,39,41	0
2	NDP	G	301	48/48	0.96	0.13	-0.10	26,38,44,49	0

6.5 Other polymers (i)

There are no such residues in this entry.