



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:23 PM GMT

PDB ID : 4C3Y  
Title : Crystal structure of 3-ketosteroid delta1-dehydrogenase from *Rhodococcus erythropolis* SQ1 in complex with 1,4-androstadiene-3,17- dione  
Authors : Rohman, A.; van Oosterwijk, N.; Thunnissen, A.M.W.H.; Dijkstra, B.W.  
Deposited on : 2013-08-28  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

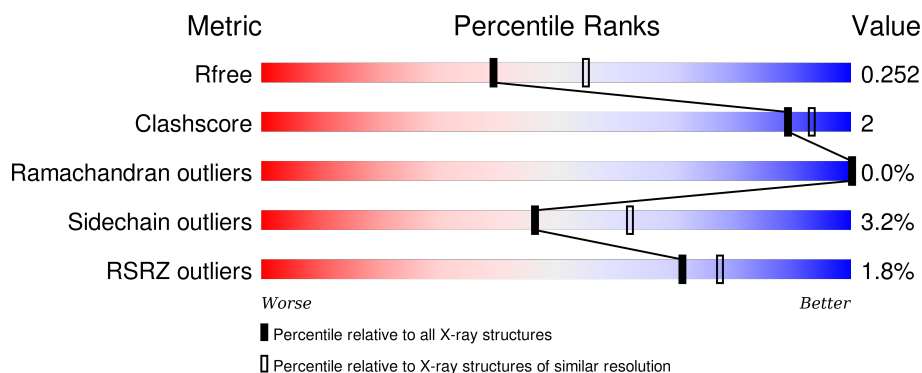
# 1 Overall quality at a glance ⓘ

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  $\geq 3$ , 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  $\leq 5\%$ . 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	530	<div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	B	530	<div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	C	530	<div> <div>2%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	D	530	<div> <div>2%</div> <div>88%</div> <div>7%</div> <div>.</div> </div>
1	E	530	<div> <div>3%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	530	
1	G	530	
1	H	530	

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
4	PG4	A	581	-	-	-	X
4	PG4	B	581	-	-	-	X
4	PG4	D	581	-	-	-	X
4	PG4	F	581	-	-	-	X
4	PG4	H	581	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31708 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-KETOSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			
1	B	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	C	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	D	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			
1	E	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			
1	F	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	G	505	Total	C	N	O	S	0	0	0
			3693	2294	643	742	14			
1	H	508	Total	C	N	O	S	0	0	0
			3712	2305	647	746	14			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
A	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
A	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
A	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
A	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
A	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
A	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
A	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
A	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
A	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
A	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
A	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
A	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
A	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02
A	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
A	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02
A	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
A	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
A	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
B	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
B	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
B	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
B	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
B	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
B	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
B	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
B	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
B	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
B	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
B	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
B	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
B	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02
B	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
B	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02
B	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
B	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02
B	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
B	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
B	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
C	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
C	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
C	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
C	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
C	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
C	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
C	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
C	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
C	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
C	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
C	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
C	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
C	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02
C	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
C	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
C	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02
C	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
C	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
C	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
D	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
D	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
D	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
D	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
D	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
D	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
D	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
D	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
D	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
D	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
D	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
D	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
D	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02
D	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
D	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02
D	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
D	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02
D	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
D	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
D	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
E	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
E	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
E	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
E	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
E	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
E	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
E	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
E	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
E	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
E	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
E	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
E	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
E	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02
E	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
E	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02
E	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
E	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02

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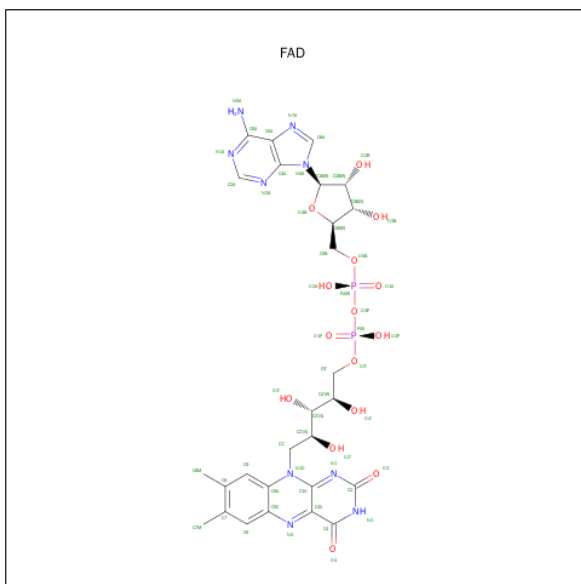
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
E	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
E	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
F	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
F	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
F	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
F	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
F	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
F	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02
F	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
F	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02
F	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
F	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02
F	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
F	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
F	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
G	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
G	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
G	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
G	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
G	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
G	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
G	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
G	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
G	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
G	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
G	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
G	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
G	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02
G	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
G	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02
G	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
G	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02
G	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
G	-1	SER	-	EXPRESSION TAG	UNP Q9RA02

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
H	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
H	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
H	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
H	-16	SER	-	EXPRESSION TAG	UNP Q9RA02
H	-15	HIS	-	EXPRESSION TAG	UNP Q9RA02
H	-14	HIS	-	EXPRESSION TAG	UNP Q9RA02
H	-13	HIS	-	EXPRESSION TAG	UNP Q9RA02
H	-12	HIS	-	EXPRESSION TAG	UNP Q9RA02
H	-11	HIS	-	EXPRESSION TAG	UNP Q9RA02
H	-10	HIS	-	EXPRESSION TAG	UNP Q9RA02
H	-9	SER	-	EXPRESSION TAG	UNP Q9RA02
H	-8	SER	-	EXPRESSION TAG	UNP Q9RA02
H	-7	GLY	-	EXPRESSION TAG	UNP Q9RA02
H	-6	LEU	-	EXPRESSION TAG	UNP Q9RA02
H	-5	VAL	-	EXPRESSION TAG	UNP Q9RA02
H	-4	PRO	-	EXPRESSION TAG	UNP Q9RA02
H	-3	ARG	-	EXPRESSION TAG	UNP Q9RA02
H	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
H	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
H	0	HIS	-	EXPRESSION TAG	UNP Q9RA02

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



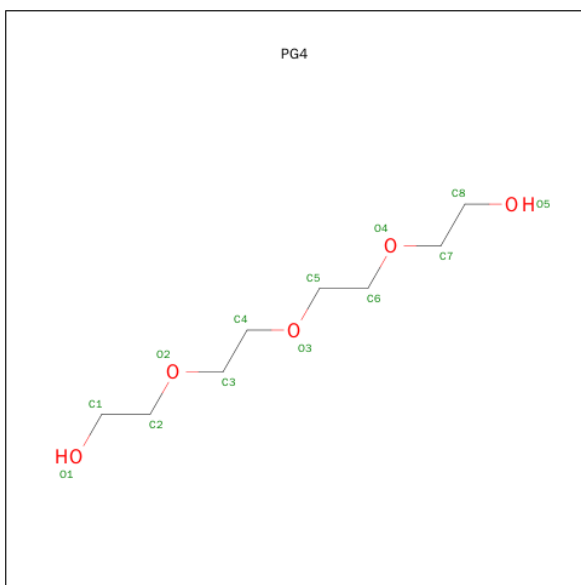


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

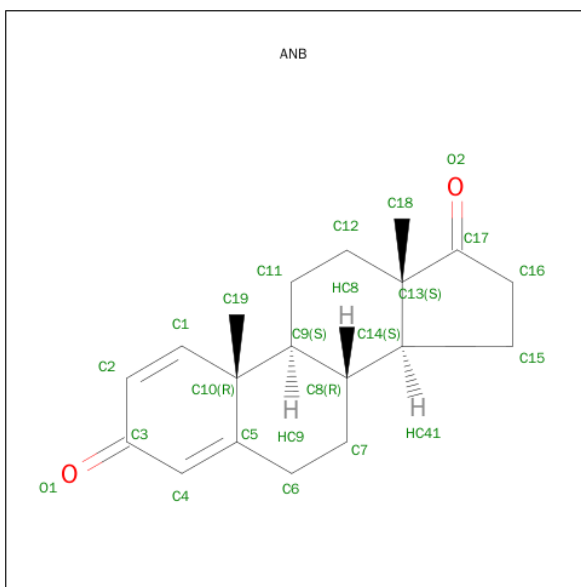
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is ANDROSTA-1,4-DIENE-3,17-DIONE (three-letter code: ANB) (formula:  $C_{19}H_{24}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 21 19 2	0	0
5	B	1	Total C O 21 19 2	0	0
5	C	1	Total C O 21 19 2	0	0
5	D	1	Total C O 21 19 2	0	0
5	E	1	Total C O 21 19 2	0	0
5	F	1	Total C O 21 19 2	0	0
5	G	1	Total C O 21 19 2	0	0
5	H	1	Total C O 21 19 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	227	Total O 227 227	0	0
6	B	201	Total O 201 201	0	0
6	C	139	Total O 139 139	0	0
6	D	180	Total O 180 180	0	0

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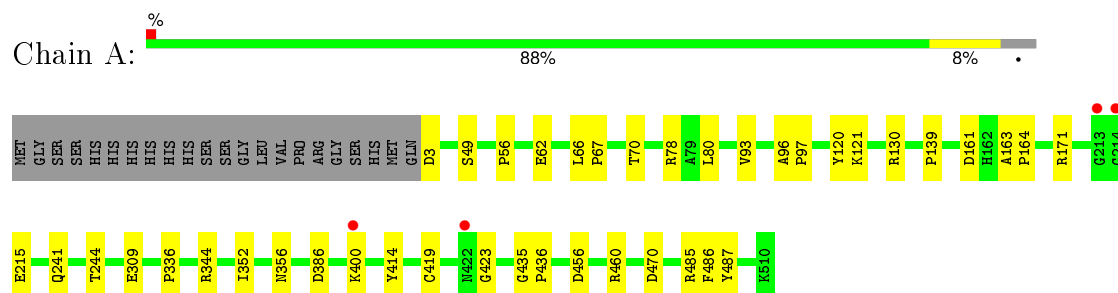
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	190	Total 190	O 190	0	0
6	F	134	Total 134	O 134	0	0
6	G	185	Total 185	O 185	0	0
6	H	158	Total 158	O 158	0	0

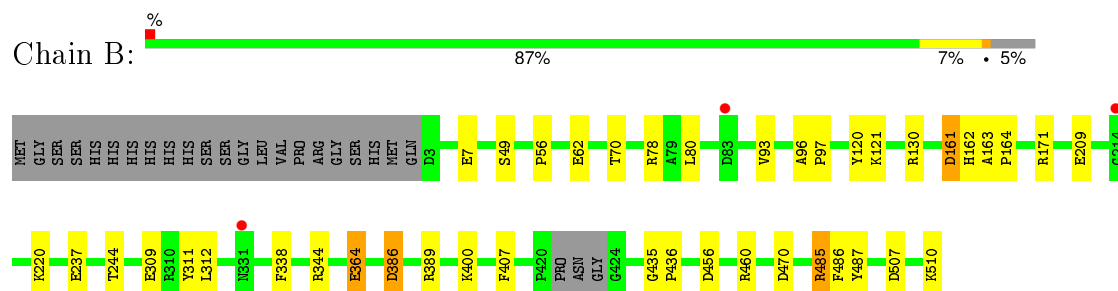
### 3 Residue-property plots [i](#)

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.

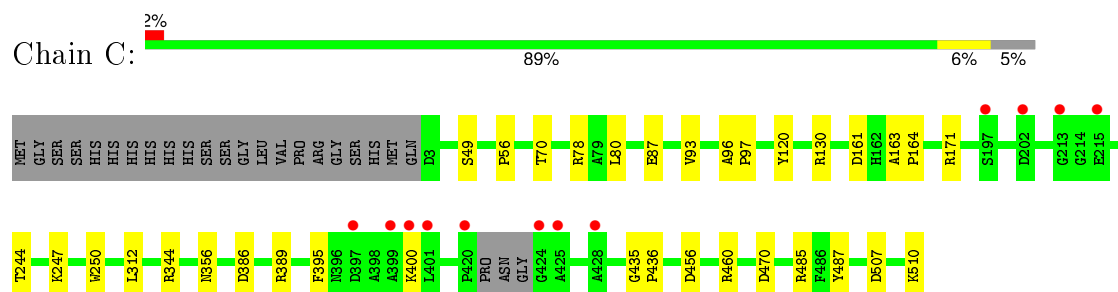
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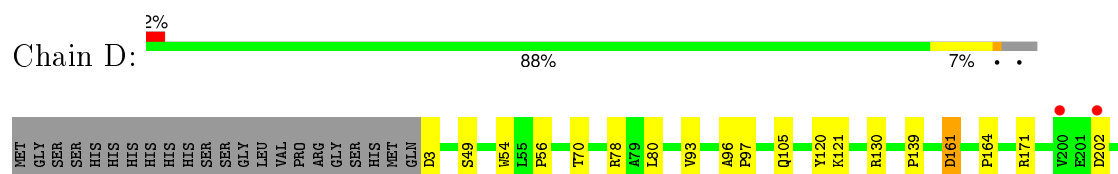
#### • Molecule 1: 3-KETOSTEROID DEHYDROGENASE

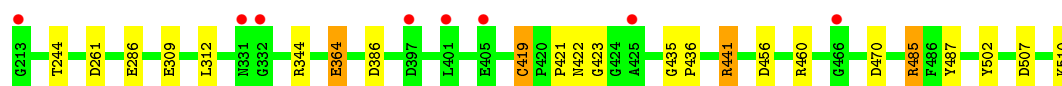


#### • Molecule 1: 3-KETOSTEROID DEHYDROGENASE

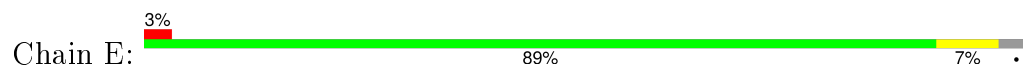


#### • Molecule 1: 3-KETOSTEROID DEHYDROGENASE

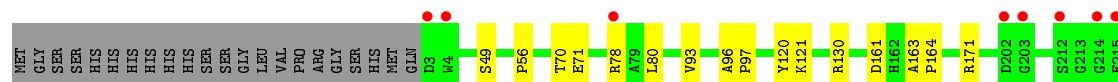
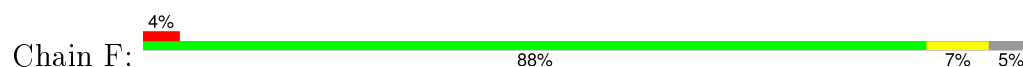




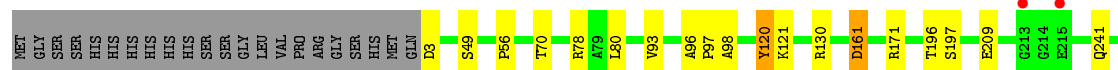
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



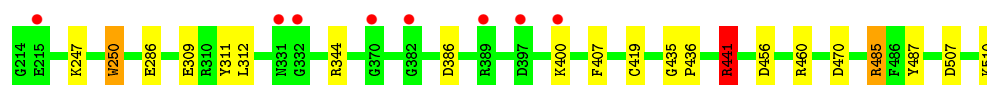
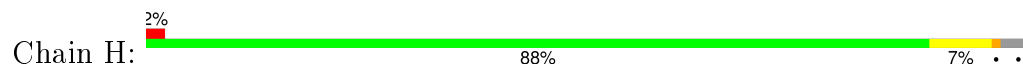
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.75Å 132.14Å 363.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 2.30 49.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.42-2.30) 99.7 (49.42-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.210 , 0.249 0.214 , 0.252	Depositor DCC
$R_{free}$ test set	11485 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 229445 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	31708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: NA, PG4, FAD, ANB

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	0.70	6/3782 (0.2%)	0.75	7/5138 (0.1%)
1	B	0.67	7/3761 (0.2%)	0.75	4/5107 (0.1%)
1	C	0.64	1/3761 (0.0%)	0.72	0/5107
1	D	0.63	4/3782 (0.1%)	0.75	5/5138 (0.1%)
1	E	0.64	4/3782 (0.1%)	0.70	1/5138 (0.0%)
1	F	0.57	0/3761	0.70	3/5107 (0.1%)
1	G	0.80	18/3761 (0.5%)	0.76	2/5107 (0.0%)
1	H	0.66	4/3782 (0.1%)	0.73	3/5138 (0.1%)
All	All	0.67	44/30172 (0.1%)	0.73	25/40980 (0.1%)

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	E	0	1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	438	TYR	CE1-CZ	9.33	1.50	1.38
1	D	502	TYR	CE1-CZ	9.17	1.50	1.38
1	G	502	TYR	CE2-CZ	9.02	1.50	1.38
1	E	502	TYR	CE1-CZ	8.00	1.49	1.38
1	A	414	TYR	CE1-CZ	7.87	1.48	1.38
1	G	120	TYR	CE1-CZ	7.70	1.48	1.38
1	G	120	TYR	CE2-CZ	7.28	1.48	1.38
1	E	502	TYR	CG-CD2	7.16	1.48	1.39
1	E	502	TYR	CE2-CZ	7.09	1.47	1.38
1	H	111	PHE	CG-CD2	6.94	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	TYR	CG-CD2	6.88	1.48	1.39
1	G	120	TYR	CG-CD1	6.68	1.47	1.39
1	D	502	TYR	CG-CD2	6.66	1.47	1.39
1	C	395	PHE	CG-CD2	6.62	1.48	1.38
1	H	111	PHE	CG-CD1	6.58	1.48	1.38
1	G	438	TYR	CG-CD1	6.50	1.47	1.39
1	A	414	TYR	CG-CD2	6.49	1.47	1.39
1	G	338	PHE	CG-CD2	6.46	1.48	1.38
1	G	502	TYR	CG-CD2	6.46	1.47	1.39
1	G	502	TYR	CG-CD1	6.42	1.47	1.39
1	E	502	TYR	CG-CD1	6.42	1.47	1.39
1	B	338	PHE	CG-CD2	6.34	1.48	1.38
1	B	338	PHE	CE2-CZ	6.25	1.49	1.37
1	G	395	PHE	CG-CD2	6.21	1.48	1.38
1	G	338	PHE	CG-CD1	6.17	1.48	1.38
1	G	338	PHE	CE1-CZ	6.16	1.49	1.37
1	D	502	TYR	CG-CD1	6.15	1.47	1.39
1	B	338	PHE	CG-CD1	6.10	1.47	1.38
1	A	486	PHE	CG-CD1	6.04	1.47	1.38
1	G	437	PHE	CG-CD1	6.01	1.47	1.38
1	A	486	PHE	CG-CD2	5.75	1.47	1.38
1	A	486	PHE	CE2-CZ	5.72	1.48	1.37
1	B	338	PHE	CE1-CZ	5.69	1.48	1.37
1	D	54	TRP	CD2-CE2	5.68	1.48	1.41
1	H	111	PHE	CE1-CZ	5.64	1.48	1.37
1	B	486	PHE	CE1-CZ	5.36	1.47	1.37
1	B	486	PHE	CE2-CZ	5.31	1.47	1.37
1	B	486	PHE	CG-CD1	5.29	1.46	1.38
1	A	486	PHE	CE1-CZ	5.24	1.47	1.37
1	H	250	TRP	CD2-CE2	5.22	1.47	1.41
1	G	437	PHE	CG-CD2	5.15	1.46	1.38
1	G	338	PHE	CE2-CZ	5.12	1.47	1.37
1	G	437	PHE	CE1-CZ	5.08	1.47	1.37
1	G	438	TYR	CG-CD2	5.07	1.45	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	386	ASP	CB-CG-OD2	9.92	127.22	118.30
1	B	389	ARG	NE-CZ-NH1	-9.37	115.61	120.30
1	D	386	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	D	419	CYS	CA-CB-SG	-7.07	101.27	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	419	CYS	CA-CB-SG	-6.99	101.43	114.00
1	H	419	CYS	CA-CB-SG	-6.82	101.73	114.00
1	A	419	CYS	CA-CB-SG	-6.72	101.90	114.00
1	F	78	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	F	441	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	486	PHE	CB-CG-CD2	6.09	125.07	120.80
1	A	215	GLU	CB-CA-C	-6.05	98.31	110.40
1	F	364	GLU	CB-CA-C	-5.96	98.49	110.40
1	H	441	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	215	GLU	CA-CB-CG	5.84	126.25	113.40
1	B	364	GLU	CB-CA-C	-5.66	99.09	110.40
1	B	389	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	A	486	PHE	CD1-CG-CD2	-5.59	111.03	118.30
1	D	364	GLU	CB-CA-C	-5.42	99.57	110.40
1	H	7	GLU	CG-CD-OE2	5.17	128.64	118.30
1	A	486	PHE	CE1-CZ-CE2	-5.10	110.83	120.00
1	D	202	ASP	CB-CG-OD2	5.03	122.83	118.30
1	G	161	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	A	241	GLN	CA-CB-CG	5.02	124.45	113.40
1	B	486	PHE	CE1-CZ-CE2	-5.02	110.97	120.00
1	G	241	GLN	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	3	ASP	Peptide

## 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	3712	0	3579	16	0
1	B	3693	0	3562	21	0
1	C	3693	0	3562	14	0
1	D	3712	0	3579	24	0
1	E	3712	0	3579	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3693	0	3562	18	0
1	G	3693	0	3562	14	0
1	H	3712	0	3579	22	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
2	E	53	0	31	1	0
2	F	53	0	31	1	0
2	G	53	0	31	1	0
2	H	53	0	31	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	13	0	18	3	0
4	B	13	0	18	5	0
4	D	13	0	18	1	0
4	E	13	0	18	1	0
4	F	13	0	18	0	0
4	H	13	0	18	1	0
5	A	21	0	24	0	0
5	B	21	0	24	0	0
5	C	21	0	24	0	0
5	D	21	0	24	0	0
5	E	21	0	24	0	0
5	F	21	0	24	0	0
5	G	21	0	24	0	0
5	H	21	0	24	0	0
6	A	227	0	0	1	0
6	B	201	0	0	3	0
6	C	139	0	0	3	0
6	D	180	0	0	4	0
6	E	190	0	0	6	0
6	F	134	0	0	4	0
6	G	185	0	0	1	0
6	H	158	0	0	2	0
All	All	31708	0	29112	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (141) 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:D:441:ARG:HG2	1:D:441:ARG:HH11	1.35	0.91
1:F:441:ARG:HH11	1:F:441:ARG:HG2	1.34	0.91
1:H:441:ARG:HG2	1:H:441:ARG:HH11	1.37	0.87
1:B:162:HIS:HB3	4:B:581:PG4:H51	1.76	0.67
1:D:485:ARG:HD3	6:D:2177:HOH:O	1.94	0.66
1:C:356:ASN:OD1	1:D:161:ASP:HB3	1.98	0.64
1:B:49:SER:HA	2:B:551:FAD:C6	2.28	0.63
1:H:485:ARG:HG3	6:H:2061:HOH:O	1.98	0.63
1:F:441:ARG:NH1	1:F:441:ARG:HG2	2.10	0.62
1:D:49:SER:HA	2:D:551:FAD:C6	2.31	0.60
1:C:507:ASP:HA	1:C:510:LYS:HE3	1.84	0.59
1:F:441:ARG:HD2	6:F:2122:HOH:O	2.02	0.58
1:B:507:ASP:HA	1:B:510:LYS:HE3	1.85	0.58
1:G:196:THR:HG22	1:G:209:GLU:O	2.03	0.58
1:D:441:ARG:HD2	6:D:2164:HOH:O	2.04	0.58
1:A:66:LEU:O	1:D:421:PRO:HB3	2.04	0.58
1:E:507:ASP:HA	1:E:510:LYS:HE3	1.85	0.57
1:D:507:ASP:HA	1:D:510:LYS:HE3	1.85	0.57
1:H:507:ASP:HA	1:H:510:LYS:HE3	1.86	0.57
1:G:507:ASP:HA	1:G:510:LYS:HE3	1.86	0.57
1:F:507:ASP:HA	1:F:510:LYS:HE3	1.85	0.57
1:E:382:GLY:HA2	6:E:2156:HOH:O	2.05	0.56
1:E:49:SER:HA	2:E:551:FAD:C6	2.37	0.55
1:H:105:GLN:NE2	6:H:2031:HOH:O	2.34	0.53
1:C:389:ARG:HG2	6:C:2123:HOH:O	2.09	0.53
1:C:49:SER:HA	2:C:551:FAD:C6	2.39	0.53
1:H:441:ARG:HH11	1:H:441:ARG:CG	2.16	0.52
1:H:286:GLU:OE1	1:H:441:ARG:NH1	2.43	0.52
1:H:96:ALA:HB3	1:H:97:PRO:HD3	1.91	0.51
1:E:361:LYS:HE3	6:E:2151:HOH:O	2.10	0.51
1:A:96:ALA:HB3	1:A:97:PRO:HD3	1.92	0.51
1:D:139:PRO:HG3	4:D:581:PG4:H42	1.91	0.51
1:F:406:GLU:HG2	6:F:2119:HOH:O	2.10	0.51
1:D:96:ALA:HB3	1:D:97:PRO:HD3	1.92	0.51
1:F:441:ARG:HH11	1:F:441:ARG:CG	2.15	0.51
1:D:456:ASP:OD2	1:D:460:ARG:HD3	2.11	0.51
1:G:456:ASP:OD2	1:G:460:ARG:HD3	2.10	0.51
1:C:456:ASP:OD2	1:C:460:ARG:HD3	2.11	0.50
1:A:336:PRO:HD2	6:A:2171:HOH:O	2.11	0.50
1:E:456:ASP:OD2	1:E:460:ARG:HD3	2.11	0.50
1:F:96:ALA:HB3	1:F:97:PRO:HD3	1.92	0.50
1:B:456:ASP:OD2	1:B:460:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:HIS:CB	4:B:581:PG4:H51	2.40	0.50
1:E:96:ALA:HB3	1:E:97:PRO:HD3	1.93	0.50
1:D:441:ARG:CG	1:D:441:ARG:HH11	2.15	0.50
1:D:286:GLU:OE1	1:D:441:ARG:NH1	2.45	0.50
1:B:386:ASP:HB2	6:B:2161:HOH:O	2.12	0.50
1:F:456:ASP:OD2	1:F:460:ARG:HD3	2.12	0.50
1:E:146:ALA:HB3	4:E:581:PG4:H72	1.93	0.50
1:D:261:ASP:HA	6:D:2095:HOH:O	2.10	0.49
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.94	0.49
1:C:96:ALA:HB3	1:C:97:PRO:HD3	1.94	0.49
1:A:456:ASP:OD2	1:A:460:ARG:HD3	2.12	0.49
1:H:456:ASP:OD2	1:H:460:ARG:HD3	2.12	0.48
1:F:49:SER:HA	2:F:551:FAD:C6	2.43	0.48
1:C:80:LEU:HD21	1:C:120:TYR:CG	2.49	0.48
1:A:67:PRO:HB3	1:D:419:CYS:O	2.13	0.48
1:F:457:VAL:HG13	6:F:2125:HOH:O	2.14	0.48
1:A:80:LEU:HD21	1:A:120:TYR:CG	2.49	0.48
1:F:286:GLU:OE1	1:F:441:ARG:NH1	2.47	0.48
1:G:49:SER:HA	2:G:551:FAD:C6	2.44	0.48
1:H:441:ARG:HG2	1:H:441:ARG:NH1	2.12	0.48
1:G:96:ALA:HB3	1:G:97:PRO:HD3	1.95	0.48
1:F:71:GLU:HG2	6:F:2021:HOH:O	2.12	0.48
1:A:435:GLY:HA2	1:A:436:PRO:C	2.35	0.47
1:E:164:PRO:HG3	6:E:2085:HOH:O	2.14	0.47
1:B:62:GLU:HA	6:B:2019:HOH:O	2.13	0.47
1:H:49:SER:HA	2:H:551:FAD:C6	2.45	0.47
6:C:2056:HOH:O	1:D:164:PRO:HG3	2.13	0.47
1:B:80:LEU:HD21	1:B:120:TYR:CG	2.50	0.47
1:F:80:LEU:HD21	1:F:120:TYR:CG	2.50	0.46
1:E:70:THR:HG23	1:E:93:VAL:CG1	2.46	0.46
1:A:62:GLU:OE2	1:D:422:ASN:OD1	2.33	0.46
1:C:70:THR:HG23	1:C:93:VAL:CG1	2.46	0.46
1:F:56:PRO:HB3	1:F:130:ARG:HD3	1.97	0.46
1:D:312:LEU:C	1:D:312:LEU:HD12	2.35	0.46
1:F:163:ALA:HB1	1:F:164:PRO:CD	2.45	0.46
1:E:151:PRO:HD2	6:E:2074:HOH:O	2.14	0.45
1:E:247:LYS:HE2	1:E:250:TRP:CH2	2.51	0.45
1:H:70:THR:HG23	1:H:93:VAL:CG1	2.46	0.45
1:B:56:PRO:HB3	1:B:130:ARG:HD3	1.98	0.45
1:H:56:PRO:HB3	1:H:130:ARG:HD3	1.97	0.45
1:F:70:THR:HG23	1:F:93:VAL:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:PRO:HB3	1:G:130:ARG:HD3	1.98	0.44
1:E:320:GLN:O	6:E:2136:HOH:O	2.21	0.44
1:B:70:THR:HG23	1:B:93:VAL:CG1	2.47	0.44
1:H:435:GLY:HA2	1:H:436:PRO:C	2.38	0.44
1:B:435:GLY:HA2	1:B:436:PRO:C	2.37	0.44
1:B:7:GLU:HG2	1:B:220:LYS:HB3	1.99	0.44
1:G:3:ASP:OD1	1:G:3:ASP:N	2.51	0.44
1:A:139:PRO:HG3	4:A:581:PG4:H42	1.99	0.44
1:D:70:THR:HG23	1:D:93:VAL:CG1	2.48	0.44
4:A:581:PG4:H52	4:A:581:PG4:O1	2.18	0.44
1:H:80:LEU:HD21	1:H:120:TYR:CG	2.52	0.44
1:E:80:LEU:HD21	1:E:120:TYR:CG	2.53	0.44
1:A:49:SER:HA	2:A:551:FAD:C6	2.47	0.44
1:A:70:THR:HG23	1:A:93:VAL:CG1	2.48	0.44
1:H:49:SER:HB2	2:H:551:FAD:C4X	2.48	0.44
1:D:80:LEU:HD21	1:D:120:TYR:CG	2.53	0.43
1:H:247:LYS:HE2	1:H:250:TRP:CH2	2.53	0.43
1:G:70:THR:HG23	1:G:93:VAL:CG1	2.49	0.43
1:C:56:PRO:HB3	1:C:130:ARG:HD3	1.99	0.43
1:E:56:PRO:HB3	1:E:130:ARG:HD3	2.00	0.43
1:D:56:PRO:HB3	1:D:130:ARG:HD3	1.99	0.43
1:B:312:LEU:HD12	1:B:312:LEU:C	2.39	0.43
1:D:435:GLY:HA2	1:D:436:PRO:C	2.39	0.43
1:A:163:ALA:HB1	1:A:164:PRO:CD	2.48	0.43
1:A:139:PRO:HB3	4:A:581:PG4:H51	2.00	0.43
1:H:163:ALA:HB1	1:H:164:PRO:CD	2.49	0.43
1:C:435:GLY:HA2	1:C:436:PRO:C	2.39	0.43
1:B:163:ALA:O	4:B:581:PG4:H41	2.18	0.43
1:D:105:GLN:HB3	6:D:2039:HOH:O	2.18	0.42
1:E:435:GLY:HA2	1:E:436:PRO:C	2.39	0.42
1:B:485:ARG:HG2	6:B:2195:HOH:O	2.20	0.42
1:H:165:GLY:O	4:H:581:PG4:H32	2.18	0.42
1:G:435:GLY:HA2	1:G:436:PRO:C	2.39	0.42
1:G:80:LEU:HD21	1:G:120:TYR:CG	2.55	0.42
1:D:49:SER:HB2	2:D:551:FAD:C4X	2.50	0.42
1:B:162:HIS:HB3	4:B:581:PG4:C5	2.47	0.42
1:B:163:ALA:HB1	1:B:164:PRO:CD	2.50	0.42
1:H:37:GLU:OE2	2:H:551:FAD:O2B	2.32	0.42
1:F:312:LEU:HD12	1:F:312:LEU:C	2.39	0.42
1:C:312:LEU:HD12	1:C:312:LEU:C	2.40	0.42
1:B:49:SER:HB2	2:B:551:FAD:C4X	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:LYS:HE2	1:G:250:TRP:CH2	2.56	0.41
1:A:356:ASN:ND2	1:B:161:ASP:HB3	2.35	0.41
1:G:98:ALA:HA	6:G:2036:HOH:O	2.20	0.41
1:G:196:THR:HG23	1:G:197:SER:N	2.35	0.41
1:E:344:ARG:HD3	6:E:2146:HOH:O	2.20	0.41
1:A:352:ILE:HD13	4:B:581:PG4:H11	2.03	0.41
1:A:56:PRO:HB3	1:A:130:ARG:HD3	2.01	0.41
1:H:311:TYR:HA	1:H:407:PHE:CZ	2.56	0.41
1:C:163:ALA:HB1	1:C:164:PRO:CD	2.51	0.41
1:D:441:ARG:NH1	1:D:441:ARG:HG2	2.11	0.41
1:F:435:GLY:HA2	1:F:436:PRO:C	2.42	0.41
1:C:87:GLU:HB2	6:C:2028:HOH:O	2.21	0.41
1:E:163:ALA:HB1	1:E:164:PRO:CD	2.51	0.40
1:H:312:LEU:HD12	1:H:312:LEU:C	2.42	0.40
1:B:311:TYR:HA	1:B:407:PHE:CZ	2.56	0.40
1:G:356:ASN:ND2	1:H:161:ASP:HB3	2.36	0.40
1:C:247:LYS:HE2	1:C:250:TRP:CH2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	506/530 (96%)	494 (98%)	11 (2%)	1 (0%)	52	64
1	B	501/530 (94%)	490 (98%)	11 (2%)	0	100	100
1	C	501/530 (94%)	490 (98%)	11 (2%)	0	100	100
1	D	506/530 (96%)	494 (98%)	11 (2%)	1 (0%)	52	64
1	E	506/530 (96%)	493 (97%)	13 (3%)	0	100	100
1	F	501/530 (94%)	490 (98%)	11 (2%)	0	100	100
1	G	501/530 (94%)	491 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	506/530 (96%)	494 (98%)	12 (2%)	0	100	100
All	All	4028/4240 (95%)	3936 (98%)	90 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	423	GLY
1	A	423	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/388 (95%)	356 (96%)	13 (4%)	43	58
1	B	367/388 (95%)	352 (96%)	15 (4%)	37	50
1	C	367/388 (95%)	357 (97%)	10 (3%)	52	70
1	D	369/388 (95%)	356 (96%)	13 (4%)	43	58
1	E	369/388 (95%)	358 (97%)	11 (3%)	48	65
1	F	367/388 (95%)	355 (97%)	12 (3%)	45	61
1	G	367/388 (95%)	357 (97%)	10 (3%)	52	70
1	H	369/388 (95%)	358 (97%)	11 (3%)	48	65
All	All	2944/3104 (95%)	2849 (97%)	95 (3%)	46	62

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	78	ARG
1	A	121	LYS
1	A	161	ASP
1	A	171	ARG
1	A	244	THR

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Mol	Chain	Res	Type
1	A	309	GLU
1	A	344	ARG
1	A	386	ASP
1	A	400	LYS
1	A	470	ASP
1	A	485	ARG
1	A	487	TYR
1	B	78	ARG
1	B	121	LYS
1	B	161	ASP
1	B	171	ARG
1	B	209	GLU
1	B	237	GLU
1	B	244	THR
1	B	309	GLU
1	B	344	ARG
1	B	364	GLU
1	B	386	ASP
1	B	400	LYS
1	B	470	ASP
1	B	485	ARG
1	B	487	TYR
1	C	78	ARG
1	C	161	ASP
1	C	171	ARG
1	C	244	THR
1	C	344	ARG
1	C	386	ASP
1	C	400	LYS
1	C	470	ASP
1	C	485	ARG
1	C	487	TYR
1	D	3	ASP
1	D	78	ARG
1	D	121	LYS
1	D	161	ASP
1	D	171	ARG
1	D	244	THR
1	D	309	GLU
1	D	344	ARG
1	D	364	GLU
1	D	441	ARG

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Mol	Chain	Res	Type
1	D	470	ASP
1	D	485	ARG
1	D	487	TYR
1	E	78	ARG
1	E	121	LYS
1	E	161	ASP
1	E	171	ARG
1	E	244	THR
1	E	309	GLU
1	E	344	ARG
1	E	400	LYS
1	E	470	ASP
1	E	485	ARG
1	E	487	TYR
1	F	121	LYS
1	F	161	ASP
1	F	171	ARG
1	F	244	THR
1	F	309	GLU
1	F	344	ARG
1	F	386	ASP
1	F	400	LYS
1	F	441	ARG
1	F	470	ASP
1	F	485	ARG
1	F	487	TYR
1	G	78	ARG
1	G	121	LYS
1	G	161	ASP
1	G	171	ARG
1	G	309	GLU
1	G	344	ARG
1	G	400	LYS
1	G	470	ASP
1	G	485	ARG
1	G	487	TYR
1	H	78	ARG
1	H	161	ASP
1	H	171	ARG
1	H	309	GLU
1	H	344	ARG
1	H	386	ASP

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Mol	Chain	Res	Type
1	H	400	LYS
1	H	441	ARG
1	H	470	ASP
1	H	485	ARG
1	H	487	TYR

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

Mol	Chain	Res	Type
1	G	328	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](#)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	FAD	A	551	-	48,58,58	1.92	8 (16%)	54,89,89	2.72	13 (24%)
4	PG4	A	581	-	12,12,12	0.88	0	11,11,11	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ANB	A	601	-	24,24,24	3.27	10 (41%)	39,39,39	2.14	12 (30%)
2	FAD	B	551	-	48,58,58	1.88	11 (22%)	54,89,89	2.11	7 (12%)
4	PG4	B	581	-	12,12,12	0.79	0	11,11,11	0.86	0
5	ANB	B	601	-	24,24,24	3.40	11 (45%)	39,39,39	1.54	10 (25%)
2	FAD	C	551	-	48,58,58	2.05	13 (27%)	54,89,89	2.55	13 (24%)
5	ANB	C	601	-	24,24,24	3.18	9 (37%)	39,39,39	1.62	7 (17%)
2	FAD	D	551	-	48,58,58	1.94	10 (20%)	54,89,89	2.49	12 (22%)
4	PG4	D	581	-	12,12,12	0.99	0	11,11,11	0.88	0
5	ANB	D	601	-	24,24,24	3.65	11 (45%)	39,39,39	2.11	12 (30%)
2	FAD	E	551	-	48,58,58	2.55	10 (20%)	54,89,89	2.61	12 (22%)
4	PG4	E	581	-	12,12,12	1.00	0	11,11,11	1.16	1 (9%)
5	ANB	E	601	-	24,24,24	3.37	10 (41%)	39,39,39	1.99	8 (20%)
2	FAD	F	551	-	48,58,58	1.64	8 (16%)	54,89,89	2.18	9 (16%)
4	PG4	F	581	-	12,12,12	1.04	0	11,11,11	0.76	1 (9%)
5	ANB	F	601	-	24,24,24	3.46	10 (41%)	39,39,39	1.87	8 (20%)
2	FAD	G	551	-	48,58,58	2.07	13 (27%)	54,89,89	2.34	10 (18%)
5	ANB	G	601	-	24,24,24	3.10	9 (37%)	39,39,39	2.07	8 (20%)
2	FAD	H	551	-	48,58,58	1.81	10 (20%)	54,89,89	2.54	11 (20%)
4	PG4	H	581	-	12,12,12	0.92	0	11,11,11	0.80	0
5	ANB	H	601	-	24,24,24	3.52	12 (50%)	39,39,39	1.51	8 (20%)

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	FAD	A	551	-	-	0/30/50/50	0/6/6/6
4	PG4	A	581	-	-	0/10/10/10	0/0/0/0
5	ANB	A	601	-	-	0/0/58/58	0/4/4/4
2	FAD	B	551	-	-	0/30/50/50	0/6/6/6
4	PG4	B	581	-	-	0/10/10/10	0/0/0/0
5	ANB	B	601	-	-	0/0/58/58	0/4/4/4
2	FAD	C	551	-	-	0/30/50/50	0/6/6/6
5	ANB	C	601	-	-	0/0/58/58	0/4/4/4
2	FAD	D	551	-	-	0/30/50/50	0/6/6/6
4	PG4	D	581	-	-	0/10/10/10	0/0/0/0
5	ANB	D	601	-	-	0/0/58/58	0/4/4/4
2	FAD	E	551	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	E	581	-	-	0/10/10/10	0/0/0/0
5	ANB	E	601	-	-	0/0/58/58	0/4/4/4
2	FAD	F	551	-	-	0/30/50/50	0/6/6/6
4	PG4	F	581	-	-	0/10/10/10	0/0/0/0
5	ANB	F	601	-	-	0/0/58/58	0/4/4/4
2	FAD	G	551	-	-	0/30/50/50	0/6/6/6
5	ANB	G	601	-	-	0/0/58/58	0/4/4/4
2	FAD	H	551	-	-	0/30/50/50	0/6/6/6
4	PG4	H	581	-	-	0/10/10/10	0/0/0/0
5	ANB	H	601	-	-	0/0/58/58	0/4/4/4

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	ANB	C13-C17	-9.93	1.38	1.52
5	H	601	ANB	C13-C17	-9.48	1.39	1.52
5	B	601	ANB	C13-C17	-8.94	1.39	1.52
5	G	601	ANB	C13-C17	-8.80	1.40	1.52
5	D	601	ANB	C10-C5	-8.77	1.41	1.51
5	E	601	ANB	C13-C17	-8.54	1.40	1.52
5	F	601	ANB	C10-C5	-8.38	1.42	1.51
5	C	601	ANB	C13-C17	-7.71	1.41	1.52
5	D	601	ANB	C13-C17	-7.62	1.41	1.52
5	F	601	ANB	C13-C17	-7.35	1.42	1.52
5	C	601	ANB	C10-C5	-7.12	1.43	1.51
2	E	551	FAD	C8M-C8	-6.86	1.37	1.51
5	F	601	ANB	C10-C1	-6.51	1.41	1.50
5	E	601	ANB	C10-C1	-6.50	1.41	1.50
5	A	601	ANB	C10-C5	-6.42	1.44	1.51
2	G	551	FAD	C7M-C7	-6.36	1.38	1.51
5	D	601	ANB	C10-C1	-6.32	1.41	1.50
5	B	601	ANB	C10-C1	-6.16	1.42	1.50
5	B	601	ANB	C10-C5	-6.11	1.44	1.51
2	D	551	FAD	C7M-C7	-5.97	1.38	1.51
5	H	601	ANB	C10-C5	-5.82	1.45	1.51
2	B	551	FAD	C7M-C7	-5.80	1.39	1.51
5	E	601	ANB	C10-C5	-5.69	1.45	1.51
2	B	551	FAD	C8M-C8	-5.60	1.39	1.51
2	G	551	FAD	C8M-C8	-5.56	1.39	1.51
2	H	551	FAD	C8M-C8	-5.39	1.40	1.51
2	A	551	FAD	C8M-C8	-5.21	1.40	1.51
2	F	551	FAD	C8M-C8	-5.11	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	ANB	C10-C1	-5.06	1.43	1.50
5	G	601	ANB	C16-C17	-4.95	1.42	1.51
2	C	551	FAD	C8M-C8	-4.91	1.41	1.51
5	B	601	ANB	C6-C5	-4.90	1.42	1.50
5	G	601	ANB	C10-C1	-4.80	1.44	1.50
5	E	601	ANB	C16-C17	-4.80	1.43	1.51
5	H	601	ANB	C6-C5	-4.78	1.42	1.50
2	C	551	FAD	C7M-C7	-4.74	1.41	1.51
2	E	551	FAD	C7M-C7	-4.62	1.41	1.51
5	H	601	ANB	C16-C17	-4.55	1.43	1.51
5	E	601	ANB	C6-C5	-4.55	1.43	1.50
5	H	601	ANB	C10-C1	-4.50	1.44	1.50
2	A	551	FAD	C10-N10	-4.41	1.34	1.39
2	F	551	FAD	C7M-C7	-4.40	1.42	1.51
2	D	551	FAD	C8M-C8	-4.26	1.42	1.51
5	F	601	ANB	C16-C17	-4.20	1.44	1.51
2	H	551	FAD	C7M-C7	-4.19	1.42	1.51
5	G	601	ANB	C10-C5	-4.18	1.47	1.51
2	H	551	FAD	C6-C5X	-4.16	1.35	1.41
5	C	601	ANB	C16-C17	-4.14	1.44	1.51
2	A	551	FAD	C7M-C7	-3.92	1.43	1.51
5	D	601	ANB	C6-C5	-3.86	1.44	1.50
5	A	601	ANB	C10-C1	-3.80	1.45	1.50
5	A	601	ANB	C6-C5	-3.74	1.44	1.50
5	B	601	ANB	C16-C17	-3.66	1.45	1.51
5	G	601	ANB	C6-C5	-3.64	1.44	1.50
2	G	551	FAD	C10-N10	-3.61	1.35	1.39
5	F	601	ANB	C6-C5	-3.57	1.44	1.50
5	D	601	ANB	C16-C17	-3.31	1.45	1.51
2	G	551	FAD	C9A-N10	-3.26	1.34	1.38
2	A	551	FAD	C5A-C4A	-3.22	1.33	1.40
5	C	601	ANB	C6-C5	-3.01	1.45	1.50
5	F	601	ANB	C2-C3	-2.95	1.39	1.45
2	E	551	FAD	C5A-C4A	-2.89	1.34	1.40
2	B	551	FAD	C5A-C4A	-2.88	1.34	1.40
5	A	601	ANB	C16-C17	-2.88	1.46	1.51
2	H	551	FAD	C5A-C4A	-2.87	1.34	1.40
2	G	551	FAD	PA-O2A	-2.76	1.43	1.54
2	H	551	FAD	C9A-C5X	-2.75	1.37	1.42
2	E	551	FAD	C10-N10	-2.65	1.36	1.39
2	D	551	FAD	C5A-C4A	-2.61	1.34	1.40
5	D	601	ANB	C2-C3	-2.59	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	551	FAD	C5A-C4A	-2.57	1.34	1.40
5	C	601	ANB	C4-C3	-2.51	1.39	1.45
2	B	551	FAD	C6-C5X	-2.45	1.38	1.41
5	B	601	ANB	C2-C3	-2.41	1.40	1.45
5	D	601	ANB	C4-C3	-2.40	1.39	1.45
2	G	551	FAD	O2'-C2'	-2.38	1.38	1.43
2	C	551	FAD	C10-N10	-2.29	1.36	1.39
2	C	551	FAD	PA-O2A	-2.28	1.45	1.54
2	B	551	FAD	PA-O2A	-2.26	1.45	1.54
5	G	601	ANB	C4-C3	-2.26	1.39	1.45
5	B	601	ANB	C4-C3	-2.21	1.39	1.45
2	D	551	FAD	PA-O2A	-2.18	1.45	1.54
2	C	551	FAD	P-O2P	-2.16	1.45	1.54
2	D	551	FAD	C9A-N10	-2.12	1.35	1.38
5	E	601	ANB	C4-C3	-2.07	1.40	1.45
2	G	551	FAD	O4B-C1B	-2.06	1.38	1.41
2	G	551	FAD	C5A-C4A	-2.05	1.35	1.40
2	B	551	FAD	C9A-C5X	-2.02	1.38	1.42
5	E	601	ANB	C2-C3	-2.02	1.41	1.45
2	F	551	FAD	C4A-N3A	-2.01	1.32	1.35
2	F	551	FAD	C5A-C4A	-2.00	1.36	1.40
5	C	601	ANB	C11-C9	2.00	1.57	1.53
2	C	551	FAD	C4A-N3A	2.09	1.38	1.35
5	G	601	ANB	O2-C17	2.15	1.25	1.21
2	G	551	FAD	C1'-N10	2.17	1.50	1.48
2	H	551	FAD	C10-N1	2.18	1.39	1.35
5	A	601	ANB	C11-C9	2.18	1.57	1.53
2	H	551	FAD	C4-N3	2.30	1.37	1.33
2	C	551	FAD	C10-N1	2.35	1.39	1.35
2	D	551	FAD	O4B-C1B	2.38	1.44	1.41
2	G	551	FAD	C4-N3	2.42	1.37	1.33
5	F	601	ANB	C7-C6	2.42	1.58	1.52
5	A	601	ANB	C12-C13	2.42	1.58	1.54
2	F	551	FAD	C10-N1	2.44	1.39	1.35
2	B	551	FAD	C2A-N3A	2.44	1.36	1.32
5	H	601	ANB	C8-C9	2.46	1.58	1.53
2	E	551	FAD	C10-N1	2.46	1.39	1.35
5	H	601	ANB	C12-C11	2.50	1.58	1.53
5	H	601	ANB	C10-C9	2.51	1.60	1.57
2	B	551	FAD	C5'-C4'	2.57	1.55	1.51
2	G	551	FAD	C10-N1	2.82	1.40	1.35
5	B	601	ANB	C11-C9	2.83	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	551	FAD	O4B-C1B	2.86	1.44	1.41
2	D	551	FAD	O3B-C3B	2.92	1.50	1.43
2	F	551	FAD	C2A-N1A	2.94	1.39	1.33
5	H	601	ANB	C12-C13	2.96	1.59	1.54
5	D	601	ANB	C8-C9	3.00	1.59	1.53
2	B	551	FAD	C1'-N10	3.02	1.51	1.48
5	B	601	ANB	C8-C9	3.03	1.59	1.53
2	A	551	FAD	C10-N1	3.07	1.40	1.35
2	H	551	FAD	C2A-N1A	3.19	1.40	1.33
5	F	601	ANB	C8-C9	3.21	1.60	1.53
5	D	601	ANB	C11-C9	3.30	1.59	1.53
5	H	601	ANB	C11-C9	3.34	1.59	1.53
2	C	551	FAD	C4-N3	3.37	1.39	1.33
2	E	551	FAD	C1'-N10	3.38	1.52	1.48
2	B	551	FAD	C2A-N1A	3.39	1.40	1.33
2	C	551	FAD	O4B-C1B	3.50	1.45	1.41
2	D	551	FAD	C4-N3	3.53	1.39	1.33
2	F	551	FAD	C2A-N3A	3.55	1.38	1.32
5	E	601	ANB	C11-C9	3.74	1.60	1.53
2	A	551	FAD	C2A-N1A	3.79	1.41	1.33
2	H	551	FAD	C2A-N3A	3.79	1.38	1.32
5	A	601	ANB	C8-C9	3.81	1.61	1.53
5	B	601	ANB	C2-C1	3.89	1.40	1.33
2	A	551	FAD	C4-N3	3.93	1.40	1.33
5	F	601	ANB	C2-C1	3.96	1.40	1.33
2	B	551	FAD	C4-N3	3.98	1.40	1.33
2	E	551	FAD	C2A-N1A	4.05	1.41	1.33
5	G	601	ANB	C2-C1	4.08	1.40	1.33
5	A	601	ANB	C4-C5	4.09	1.39	1.34
2	F	551	FAD	C4-N3	4.09	1.40	1.33
5	A	601	ANB	C2-C1	4.31	1.41	1.33
5	E	601	ANB	C2-C1	4.40	1.41	1.33
5	H	601	ANB	C2-C1	4.41	1.41	1.33
2	E	551	FAD	C4-N3	4.51	1.41	1.33
2	G	551	FAD	C2A-N1A	4.51	1.42	1.33
2	G	551	FAD	C2A-N3A	4.62	1.40	1.32
5	D	601	ANB	C2-C1	4.68	1.41	1.33
2	D	551	FAD	C2A-N1A	4.69	1.42	1.33
2	D	551	FAD	C2A-N3A	4.72	1.40	1.32
5	C	601	ANB	C2-C1	4.73	1.41	1.33
5	C	601	ANB	C4-C5	4.93	1.40	1.34
2	A	551	FAD	C2A-N3A	5.09	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	551	FAD	C1'-N10	5.14	1.53	1.48
5	G	601	ANB	C4-C5	5.17	1.41	1.34
5	E	601	ANB	C4-C5	5.21	1.41	1.34
5	B	601	ANB	C4-C5	5.22	1.41	1.34
2	C	551	FAD	C2A-N1A	5.23	1.43	1.33
2	C	551	FAD	C2A-N3A	5.52	1.42	1.32
2	E	551	FAD	C2A-N3A	5.87	1.42	1.32
5	H	601	ANB	C4-C5	5.96	1.42	1.34
5	F	601	ANB	C4-C5	6.10	1.42	1.34
5	D	601	ANB	C4-C5	6.97	1.43	1.34
2	E	551	FAD	O4B-C1B	10.67	1.54	1.41

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	551	FAD	N3A-C2A-N1A	-14.11	118.09	128.89
2	E	551	FAD	N3A-C2A-N1A	-13.81	118.32	128.89
2	H	551	FAD	N3A-C2A-N1A	-13.11	118.86	128.89
2	D	551	FAD	N3A-C2A-N1A	-12.80	119.09	128.89
2	C	551	FAD	N3A-C2A-N1A	-12.77	119.12	128.89
2	G	551	FAD	N3A-C2A-N1A	-12.04	119.67	128.89
2	B	551	FAD	N3A-C2A-N1A	-11.54	120.06	128.89
2	F	551	FAD	N3A-C2A-N1A	-11.28	120.25	128.89
2	C	551	FAD	P-O3P-PA	-6.18	115.38	132.73
5	F	601	ANB	C19-C10-C9	-6.08	107.91	111.73
2	A	551	FAD	C1B-N9A-C4A	-5.87	118.08	126.94
2	C	551	FAD	C1B-N9A-C4A	-5.47	118.69	126.94
5	D	601	ANB	C19-C10-C9	-4.92	108.64	111.73
2	E	551	FAD	C1B-N9A-C4A	-4.56	120.07	126.94
5	D	601	ANB	C2-C3-C4	-4.31	112.42	117.12
2	D	551	FAD	C1B-N9A-C4A	-4.30	120.46	126.94
2	H	551	FAD	C1B-N9A-C4A	-4.20	120.61	126.94
2	D	551	FAD	C4B-O4B-C1B	-4.06	105.26	109.72
5	E	601	ANB	C6-C5-C4	-4.01	115.81	120.89
5	D	601	ANB	C7-C8-C9	-3.86	105.84	110.46
5	A	601	ANB	C13-C14-C8	-3.82	109.01	113.12
2	E	551	FAD	C4B-O4B-C1B	-3.77	105.57	109.72
5	A	601	ANB	C16-C15-C14	-3.76	96.74	103.08
2	G	551	FAD	C4B-O4B-C1B	-3.70	105.66	109.72
2	H	551	FAD	P-O3P-PA	-3.70	122.35	132.73
5	G	601	ANB	C19-C10-C9	-3.66	109.43	111.73
2	D	551	FAD	P-O3P-PA	-3.56	122.72	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	601	ANB	C6-C5-C4	-3.54	116.39	120.89
5	C	601	ANB	C15-C14-C13	-3.46	100.70	104.06
5	E	601	ANB	C10-C9-C8	-3.31	108.92	111.97
5	E	601	ANB	C13-C14-C8	-3.20	109.67	113.12
2	C	551	FAD	C4X-C4-N3	-3.15	119.28	123.59
5	F	601	ANB	C15-C14-C13	-3.09	101.05	104.06
5	B	601	ANB	C13-C14-C8	-3.03	109.86	113.12
5	A	601	ANB	C14-C13-C17	-3.03	96.77	100.56
5	G	601	ANB	O1-C3-C4	-3.02	117.00	121.40
5	G	601	ANB	C15-C14-C13	-3.01	101.13	104.06
5	B	601	ANB	C19-C10-C9	-2.95	109.88	111.73
2	F	551	FAD	P-O3P-PA	-2.90	124.57	132.73
2	H	551	FAD	C2B-C1B-N9A	-2.90	109.87	114.29
2	G	551	FAD	O4'-C4'-C3'	-2.88	101.78	109.02
5	F	601	ANB	C2-C3-C4	-2.86	114.00	117.12
5	A	601	ANB	C6-C5-C4	-2.84	117.28	120.89
2	E	551	FAD	O4'-C4'-C3'	-2.82	101.94	109.02
2	E	551	FAD	C4X-C4-N3	-2.82	119.74	123.59
5	A	601	ANB	O2-C17-C13	-2.81	121.76	125.93
5	D	601	ANB	C6-C7-C8	-2.78	107.01	111.67
5	C	601	ANB	C16-C15-C14	-2.74	98.46	103.08
5	D	601	ANB	O2-C17-C13	-2.71	121.92	125.93
5	H	601	ANB	C12-C13-C14	-2.70	104.95	108.99
2	F	551	FAD	C2B-C1B-N9A	-2.70	110.17	114.29
5	C	601	ANB	C19-C10-C9	-2.70	110.04	111.73
5	A	601	ANB	C10-C5-C4	-2.69	120.54	122.31
5	C	601	ANB	C6-C5-C4	-2.69	117.47	120.89
2	H	551	FAD	C4X-C4-N3	-2.67	119.93	123.59
2	B	551	FAD	P-O3P-PA	-2.65	125.29	132.73
2	C	551	FAD	O3B-C3B-C2B	-2.54	103.57	111.83
5	A	601	ANB	C12-C13-C17	-2.53	112.30	116.60
4	E	581	PG4	C7-O4-C6	-2.47	102.69	113.31
2	F	551	FAD	C4X-C4-N3	-2.43	120.27	123.59
2	A	551	FAD	C4X-C4-N3	-2.42	120.28	123.59
5	E	601	ANB	C19-C10-C1	-2.41	98.78	107.52
2	G	551	FAD	C4-C4X-C10	-2.41	118.40	119.94
2	D	551	FAD	C4X-C4-N3	-2.39	120.32	123.59
5	H	601	ANB	C14-C13-C17	-2.39	97.57	100.56
2	H	551	FAD	O3P-P-O5'	-2.37	96.66	102.94
2	B	551	FAD	C4X-C4-N3	-2.36	120.36	123.59
2	A	551	FAD	C9A-C5X-N5	-2.34	118.90	122.36
2	C	551	FAD	O4B-C4B-C5B	-2.33	100.98	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	601	ANB	C7-C8-C9	-2.33	107.67	110.46
2	A	551	FAD	P-O3P-PA	-2.32	126.20	132.73
5	D	601	ANB	C16-C15-C14	-2.32	99.17	103.08
5	D	601	ANB	C13-C14-C8	-2.30	110.64	113.12
2	A	551	FAD	C2B-C1B-N9A	-2.30	110.78	114.29
2	H	551	FAD	O3B-C3B-C2B	-2.29	104.36	111.83
5	H	601	ANB	C7-C8-C9	-2.29	107.72	110.46
5	H	601	ANB	C10-C9-C8	-2.25	109.90	111.97
2	G	551	FAD	C4X-C4-N3	-2.25	120.51	123.59
5	B	601	ANB	C6-C7-C8	-2.25	107.90	111.67
5	G	601	ANB	C1-C2-C3	-2.25	119.32	121.44
5	A	601	ANB	C1-C2-C3	-2.23	119.34	121.44
2	F	551	FAD	C1B-N9A-C4A	-2.22	123.58	126.94
5	C	601	ANB	C19-C10-C5	-2.22	105.73	108.63
5	B	601	ANB	C16-C15-C14	-2.19	99.39	103.08
2	G	551	FAD	C2B-C1B-N9A	-2.19	110.95	114.29
5	B	601	ANB	C6-C5-C4	-2.18	118.12	120.89
2	D	551	FAD	O3P-P-O5'	-2.16	97.20	102.94
5	B	601	ANB	O2-C17-C13	-2.16	122.73	125.93
5	H	601	ANB	C6-C7-C8	-2.15	108.08	111.67
5	A	601	ANB	C10-C9-C8	-2.14	110.00	111.97
2	B	551	FAD	C2B-C1B-N9A	-2.13	111.03	114.29
2	A	551	FAD	C4X-C10-N10	-2.09	119.29	120.52
5	B	601	ANB	C15-C14-C13	-2.07	102.05	104.06
5	G	601	ANB	C10-C5-C4	-2.07	120.95	122.31
2	G	551	FAD	C4-C4X-N5	2.07	121.23	118.72
2	F	551	FAD	C1'-N10-C9A	2.08	121.20	118.86
5	D	601	ANB	C9-C10-C5	2.09	109.95	107.51
4	F	581	PG4	C7-O4-C6	2.13	122.46	113.31
5	D	601	ANB	C18-C13-C17	2.13	109.49	105.19
2	C	551	FAD	O3'-C3'-C2'	2.17	114.21	108.75
2	E	551	FAD	O3'-C3'-C2'	2.17	114.22	108.75
2	A	551	FAD	O2P-P-O3P	2.19	115.02	105.09
5	B	601	ANB	C18-C13-C14	2.20	116.52	112.94
2	C	551	FAD	C5X-C9A-N10	2.21	119.30	117.62
5	F	601	ANB	C9-C10-C5	2.23	110.11	107.51
2	D	551	FAD	O4B-C1B-N9A	2.33	112.97	108.10
5	G	601	ANB	C1-C10-C5	2.36	114.30	111.75
5	A	601	ANB	C18-C13-C17	2.36	109.96	105.19
5	F	601	ANB	O1-C3-C4	2.38	124.87	121.40
2	C	551	FAD	C4X-C10-N10	2.40	121.93	120.52
2	G	551	FAD	C5X-C9A-N10	2.41	119.45	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	601	ANB	C16-C17-C13	2.43	111.05	108.64
2	E	551	FAD	C2B-C3B-C4B	2.46	107.67	102.61
5	C	601	ANB	C18-C13-C17	2.50	110.24	105.19
5	E	601	ANB	C18-C13-C17	2.53	110.29	105.19
2	F	551	FAD	O4B-C1B-N9A	2.53	113.40	108.10
5	D	601	ANB	C5-C4-C3	2.54	125.22	122.76
2	H	551	FAD	O3'-C3'-C4'	2.54	115.16	108.75
5	H	601	ANB	C16-C17-C13	2.55	111.17	108.64
5	A	601	ANB	C1-C10-C5	2.57	114.53	111.75
2	B	551	FAD	O4B-C1B-N9A	2.60	113.54	108.10
2	D	551	FAD	C4-C4X-N5	2.63	121.91	118.72
5	F	601	ANB	C18-C13-C17	2.63	110.49	105.19
2	A	551	FAD	O2A-PA-O3P	2.65	117.11	105.09
2	C	551	FAD	C4X-N5-C5X	2.65	119.81	116.76
2	D	551	FAD	C1'-N10-C9A	2.71	121.91	118.86
2	E	551	FAD	C5X-C9A-N10	2.74	119.70	117.62
5	E	601	ANB	C9-C10-C5	2.80	110.78	107.51
2	C	551	FAD	C1'-N10-C9A	2.83	122.03	118.86
5	B	601	ANB	C16-C17-C13	2.86	111.47	108.64
2	A	551	FAD	C4X-N5-C5X	2.88	120.07	116.76
2	H	551	FAD	C1'-N10-C9A	2.91	122.13	118.86
5	D	601	ANB	C6-C5-C10	2.96	118.28	115.82
2	H	551	FAD	C4X-N5-C5X	2.97	120.18	116.76
2	C	551	FAD	C1'-C2'-C3'	3.05	118.53	109.82
2	E	551	FAD	C4X-N5-C5X	3.08	120.31	116.76
2	G	551	FAD	O2A-PA-O3P	3.10	119.16	105.09
5	H	601	ANB	C18-C13-C14	3.23	118.19	112.94
5	H	601	ANB	C6-C5-C10	3.26	118.54	115.82
2	B	551	FAD	C4X-N5-C5X	3.27	120.53	116.76
2	E	551	FAD	O2A-PA-O3P	3.34	120.27	105.09
2	A	551	FAD	C1'-N10-C9A	3.35	122.62	118.86
2	E	551	FAD	C1'-N10-C9A	3.51	122.80	118.86
2	D	551	FAD	C4X-C10-N10	3.54	122.61	120.52
2	A	551	FAD	C5X-C9A-N10	3.91	120.59	117.62
2	F	551	FAD	C4X-N5-C5X	4.14	121.52	116.76
2	D	551	FAD	C4X-N5-C5X	4.21	121.60	116.76
2	D	551	FAD	C4-N3-C2	4.35	119.01	115.25
5	B	601	ANB	C6-C5-C10	4.56	119.61	115.82
5	F	601	ANB	C6-C5-C10	4.58	119.64	115.82
2	F	551	FAD	C4-N3-C2	4.87	119.46	115.25
5	C	601	ANB	C6-C5-C10	5.11	120.08	115.82
2	B	551	FAD	C4-N3-C2	5.19	119.74	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	ANB	C16-C17-C13	5.23	113.83	108.64
2	C	551	FAD	C4-N3-C2	5.47	119.98	115.25
2	E	551	FAD	C4-N3-C2	6.15	120.56	115.25
2	H	551	FAD	C4-N3-C2	6.63	120.98	115.25
5	A	601	ANB	C6-C5-C10	7.40	121.98	115.82
5	E	601	ANB	C6-C5-C10	7.52	122.08	115.82
2	A	551	FAD	C4-N3-C2	7.60	121.82	115.25
2	G	551	FAD	C4-N3-C2	7.78	121.97	115.25
5	G	601	ANB	C6-C5-C10	8.12	122.58	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	551	FAD	1	0
4	A	581	PG4	3	0
2	B	551	FAD	2	0
4	B	581	PG4	5	0
2	C	551	FAD	1	0
2	D	551	FAD	2	0
4	D	581	PG4	1	0
2	E	551	FAD	1	0
4	E	581	PG4	1	0
2	F	551	FAD	1	0
2	G	551	FAD	1	0
2	H	551	FAD	3	0
4	H	581	PG4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	508/530 (95%)	0.00	4 (0%) 87 90	21, 35, 55, 99	0
1	B	505/530 (95%)	-0.01	3 (0%) 90 93	22, 36, 62, 103	0
1	C	505/530 (95%)	0.13	12 (2%) 62 71	25, 42, 64, 96	0
1	D	508/530 (95%)	0.12	10 (1%) 68 75	26, 40, 64, 89	0
1	E	508/530 (95%)	0.14	14 (2%) 56 66	26, 40, 68, 122	0
1	F	505/530 (95%)	0.18	19 (3%) 44 53	24, 45, 70, 105	0
1	G	505/530 (95%)	-0.08	2 (0%) 93 95	22, 35, 56, 85	0
1	H	508/530 (95%)	0.08	10 (1%) 68 75	21, 36, 62, 117	0
All	All	4052/4240 (95%)	0.07	74 (1%) 71 78	21, 39, 64, 122	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	331	ASN	7.1
1	E	422	ASN	6.3
1	B	331	ASN	5.9
1	F	331	ASN	5.8
1	G	213	GLY	4.6
1	D	213	GLY	4.3
1	E	3	ASP	4.0
1	C	425	ALA	3.8
1	H	400	LYS	3.7
1	F	332	GLY	3.7
1	C	420	PRO	3.5
1	C	215	GLU	3.5
1	D	401	LEU	3.5
1	H	382	GLY	3.2
1	A	422	ASN	3.2
1	F	424	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	215	GLU	3.2
1	E	4	TRP	3.2
1	C	213	GLY	3.1
1	E	213	GLY	3.1
1	F	203	GLY	3.1
1	H	3	ASP	3.1
1	C	400	LYS	3.0
1	F	4	TRP	3.0
1	E	400	LYS	3.0
1	E	215	GLU	2.9
1	D	425	ALA	2.8
1	E	218	ARG	2.8
1	F	386	ASP	2.8
1	D	466	GLY	2.7
1	D	202	ASP	2.7
1	F	425	ALA	2.7
1	C	397	ASP	2.6
1	D	331	ASN	2.6
1	F	401	LEU	2.6
1	C	401	LEU	2.5
1	C	197	SER	2.5
1	H	389	ARG	2.5
1	E	5	THR	2.5
1	E	425	ALA	2.5
1	D	332	GLY	2.5
1	H	213	GLY	2.5
1	H	215	GLU	2.5
1	C	399	ALA	2.4
1	E	202	ASP	2.4
1	G	215	GLU	2.4
1	A	214	GLY	2.4
1	F	397	ASP	2.4
1	F	202	ASP	2.4
1	H	332	GLY	2.4
1	F	403	VAL	2.4
1	F	3	ASP	2.3
1	F	400	LYS	2.3
1	D	397	ASP	2.3
1	A	213	GLY	2.3
1	H	397	ASP	2.3
1	F	434	ASN	2.3
1	D	200	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	400	LYS	2.2
1	C	424	GLY	2.2
1	D	405	GLU	2.2
1	E	423	GLY	2.2
1	H	370	GLY	2.2
1	E	214	GLY	2.2
1	B	214	GLY	2.1
1	F	399	ALA	2.1
1	F	214	GLY	2.1
1	E	84	ALA	2.1
1	F	212	SER	2.1
1	C	202	ASP	2.1
1	F	78	ARG	2.0
1	B	83	ASP	2.0
1	C	428	ALA	2.0
1	E	199	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PG4	F	581	13/13	0.63	0.35	10.81	53,72,85,87	0
4	PG4	B	581	13/13	0.80	0.27	4.93	60,72,78,78	0
4	PG4	D	581	13/13	0.80	0.21	3.34	55,59,63,64	0
4	PG4	H	581	13/13	0.88	0.17	2.68	52,56,65,71	0
4	PG4	A	581	13/13	0.84	0.19	2.23	48,52,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PG4	E	581	13/13	0.84	0.18	1.87	58,62,66,68	0
5	ANB	H	601	21/21	0.90	0.19	1.44	39,42,46,47	0
5	ANB	A	601	21/21	0.90	0.17	1.17	38,51,53,53	0
5	ANB	B	601	21/21	0.92	0.15	1.06	38,51,54,55	0
5	ANB	C	601	21/21	0.91	0.14	0.74	39,42,47,48	0
5	ANB	D	601	21/21	0.93	0.17	0.64	33,42,44,46	0
5	ANB	E	601	21/21	0.91	0.14	0.39	37,51,57,58	0
5	ANB	F	601	21/21	0.93	0.14	0.11	39,44,48,51	0
2	FAD	G	551	53/53	0.97	0.12	-0.06	26,30,34,39	0
5	ANB	G	601	21/21	0.92	0.12	-0.16	30,38,43,44	0
2	FAD	A	551	53/53	0.96	0.12	-0.43	28,32,39,44	0
2	FAD	F	551	53/53	0.97	0.12	-0.58	29,36,40,45	0
2	FAD	H	551	53/53	0.97	0.12	-0.59	23,27,32,33	0
2	FAD	E	551	53/53	0.96	0.12	-0.66	27,33,36,37	0
2	FAD	B	551	53/53	0.97	0.12	-0.67	25,32,37,38	0
2	FAD	C	551	53/53	0.97	0.11	-0.89	29,34,39,40	0
2	FAD	D	551	53/53	0.96	0.10	-1.03	28,37,41,46	0
3	NA	E	561	1/1	0.98	0.10	-2.36	30,30,30,30	0
3	NA	C	561	1/1	0.95	0.08	-3.34	33,33,33,33	0
3	NA	G	561	1/1	0.98	0.07	-4.01	25,25,25,25	0
3	NA	A	561	1/1	0.98	0.06	-4.53	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.