



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:33 am GMT

PDB ID : 4C3X
Title : Crystal structure of 3-ketosteroid delta1-dehydrogenase from Rhodococcus erythropolis SQ1
Authors : Rohman, A.; van Oosterwijk, N.; Thunnissen, A.M.W.H.; Dijkstra, B.W.
Deposited on : 2013-08-28
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

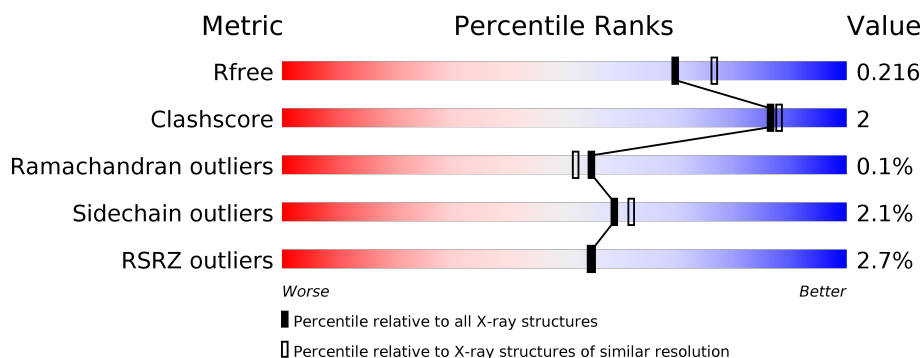
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



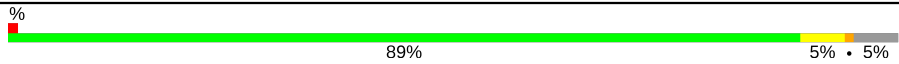
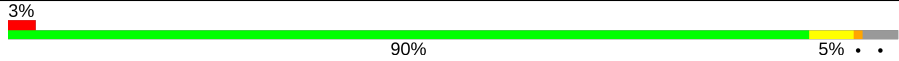
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 $\leq 5\%$. 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>2%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>• •</div> </div> </div>
1	B	530	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>• 5%</div> </div> </div>
1	C	530	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>
1	D	530	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>• •</div> </div> </div>
1	E	530	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>• •</div> </div> </div>
1	F	530	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>• 5%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	CL	B	571	-	-	-	X
5	PG4	A	581	-	-	-	X
5	PG4	A	582	-	-	-	X
5	PG4	A	583	-	-	-	X
5	PG4	B	581	-	-	-	X
5	PG4	B	582	-	-	-	X
5	PG4	C	581	-	-	-	X
5	PG4	C	582	-	-	-	X
5	PG4	D	581	-	-	-	X
5	PG4	D	582	-	-	-	X
5	PG4	E	581	-	-	-	X
5	PG4	E	582	-	-	-	X
5	PG4	E	583	-	-	-	X
5	PG4	F	581	-	-	-	X
5	PG4	G	581	-	-	-	X
5	PG4	G	582	-	-	-	X
5	PG4	H	581	-	-	-	X
5	PG4	H	582	-	-	-	X
6	SUC	B	591	-	-	-	X
6	SUC	B	592	-	-	-	X
6	SUC	D	592	-	-	-	X
6	SUC	F	591	-	-	-	X
6	SUC	H	592	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33549 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

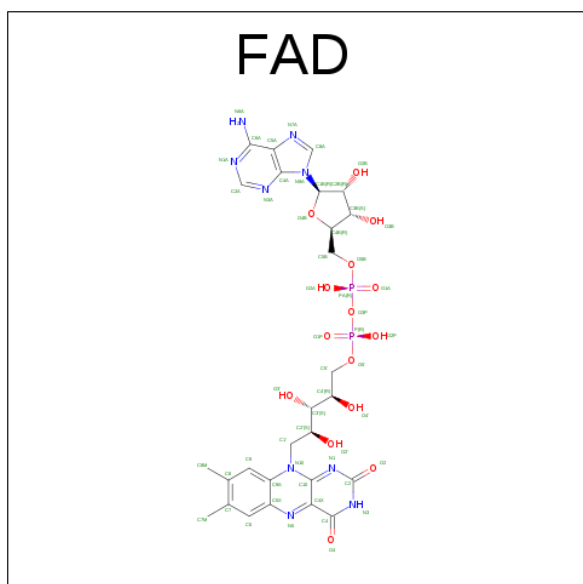
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP Q9RA02
E	-1	SER	-	EXPRESSION TAG	UNP Q9RA02
E	0	HIS	-	EXPRESSION TAG	UNP Q9RA02
F	-19	MET	-	EXPRESSION TAG	UNP Q9RA02
F	-18	GLY	-	EXPRESSION TAG	UNP Q9RA02
F	-17	SER	-	EXPRESSION TAG	UNP Q9RA02
F	-16	SER	-	EXPRESSION TAG	UNP 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

Continued on next page...

Continued from previous page...

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

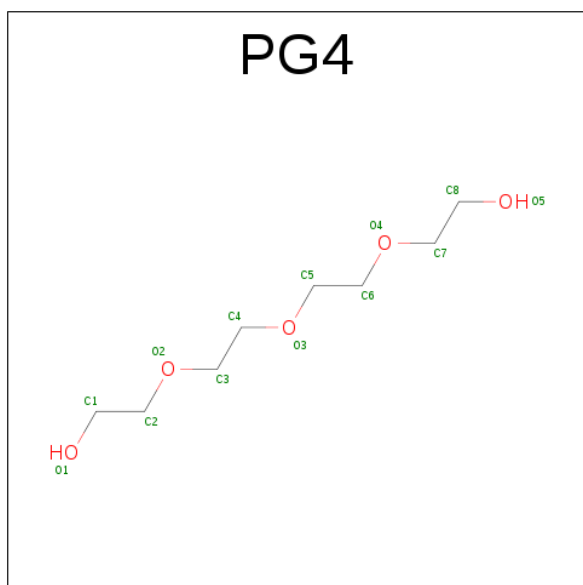
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



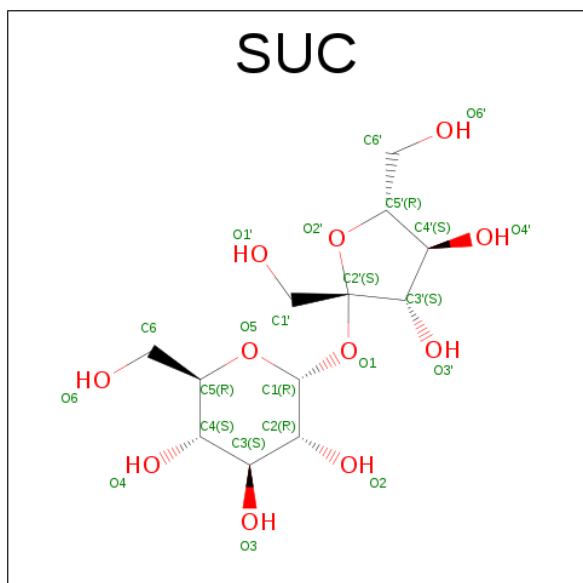
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			13	8	5		
5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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			23	12	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 23 12 11	0	0
6	B	1	Total C O 23 12 11	0	0
6	C	1	Total C O 23 12 11	0	0
6	D	1	Total C O 23 12 11	0	0
6	D	1	Total C O 23 12 11	0	0
6	E	1	Total C O 23 12 11	0	0
6	F	1	Total C O 23 12 11	0	0
6	F	1	Total C O 23 12 11	0	0
6	G	1	Total C O 23 12 11	0	0
6	H	1	Total C O 23 12 11	0	0
6	H	1	Total C O 23 12 11	0	0

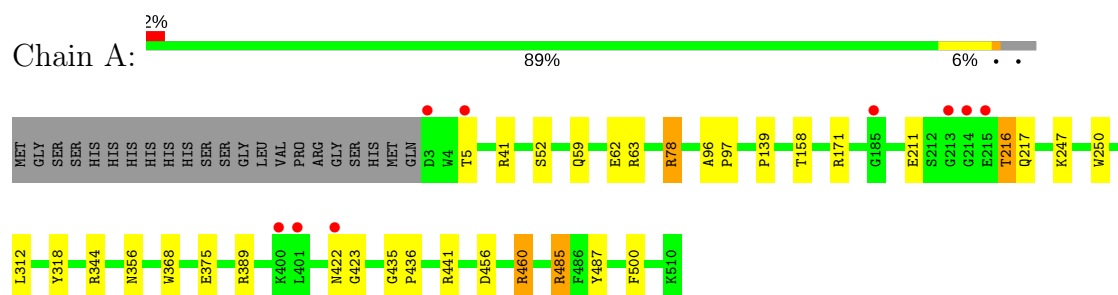
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	473	Total O 473 473	0	0
7	B	405	Total O 405 405	0	0
7	C	315	Total O 315 315	0	0
7	D	321	Total O 321 321	0	0
7	E	359	Total O 359 359	0	0
7	F	296	Total O 296 296	0	0
7	G	440	Total O 440 440	0	0
7	H	361	Total O 361 361	0	0

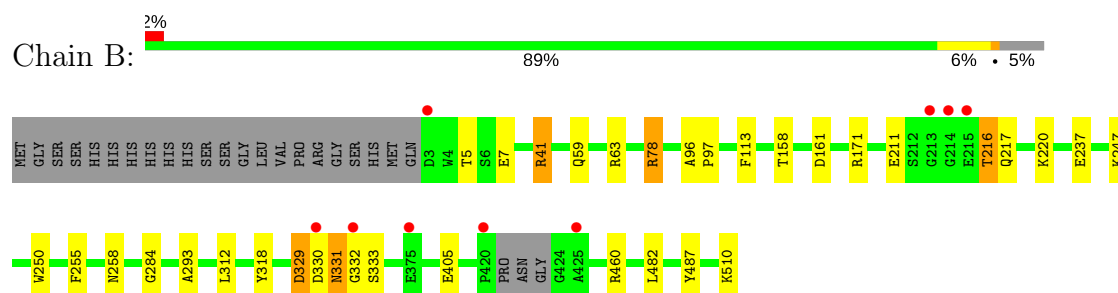
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

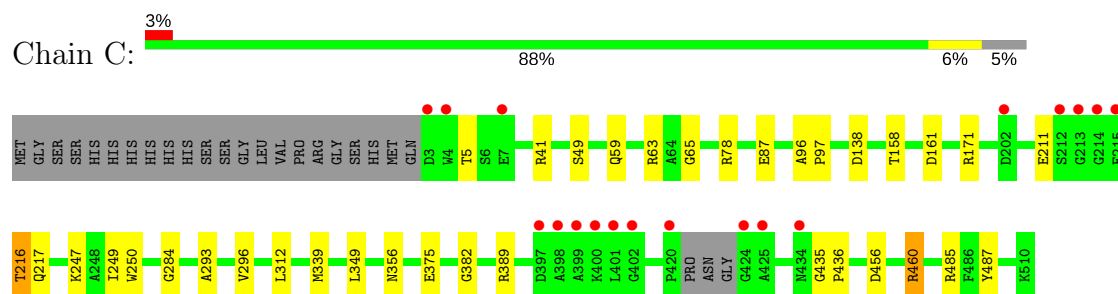
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



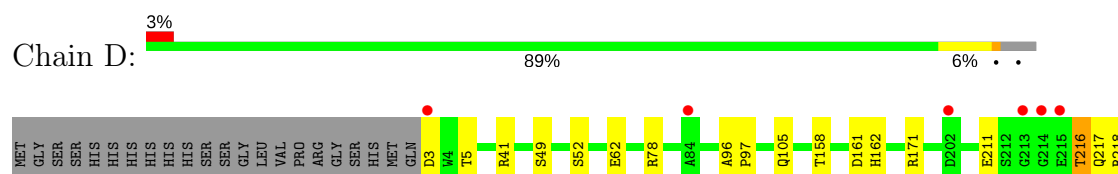
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE

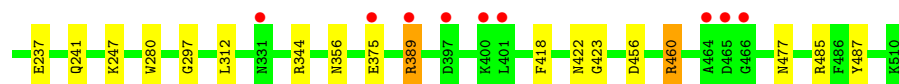


• Molecule 1: 3-KETOSTEROID DEHYDROGENASE

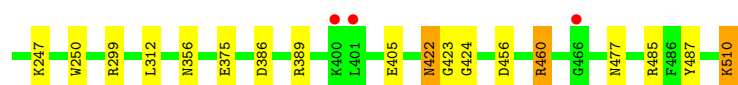
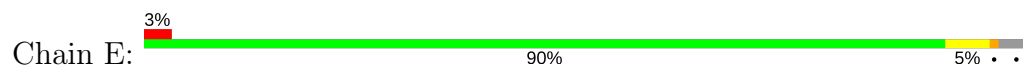


• Molecule 1: 3-KETOSTEROID DEHYDROGENASE

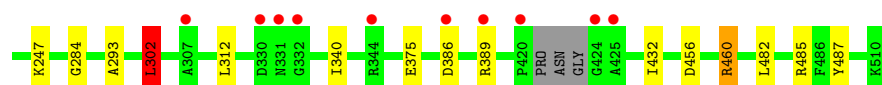
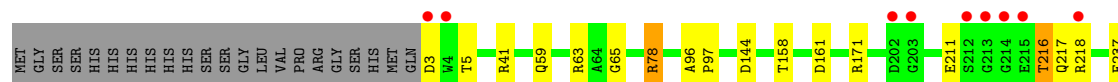




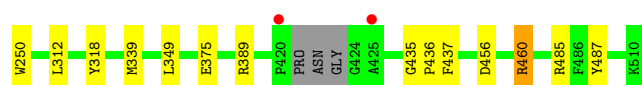
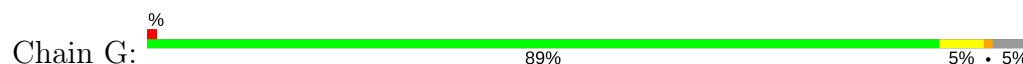
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



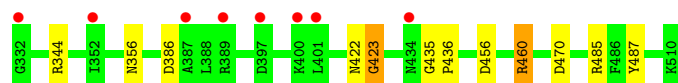
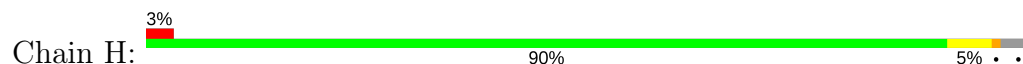
• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



• Molecule 1: 3-KETOSTEROID DEHYDROGENASE



• 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, α , β , γ	107.39Å 131.62Å 363.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.00 49.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.26-2.00) 99.8 (49.26-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.177 , 0.208 0.186 , 0.216	Depositor DCC
R_{free} test set	17445 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33549	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, PG4, SUC, FAD, CL

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	0.76	4/3782 (0.1%)	1.02	7/5138 (0.1%)
1	B	0.75	1/3761 (0.0%)	0.89	11/5107 (0.2%)
1	C	0.65	1/3761 (0.0%)	0.96	7/5107 (0.1%)
1	D	0.66	1/3782 (0.0%)	0.82	7/5138 (0.1%)
1	E	0.68	1/3782 (0.0%)	0.81	8/5138 (0.2%)
1	F	0.63	0/3761	1.01	11/5107 (0.2%)
1	G	0.76	6/3761 (0.2%)	0.82	6/5107 (0.1%)
1	H	0.72	1/3782 (0.0%)	0.99	9/5138 (0.2%)
All	All	0.70	15/30172 (0.0%)	0.92	66/40980 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	120	TYR	CG-CD1	7.88	1.49	1.39
1	G	437	PHE	CG-CD1	6.82	1.49	1.38
1	B	405	GLU	CG-CD	6.35	1.61	1.51
1	H	41	ARG	CZ-NH1	6.28	1.41	1.33
1	G	120	TYR	CE1-CZ	6.24	1.46	1.38
1	G	120	TYR	CE2-CZ	6.22	1.46	1.38
1	A	500	PHE	CG-CD2	5.89	1.47	1.38
1	A	500	PHE	CE2-CZ	5.83	1.48	1.37
1	G	437	PHE	CE1-CZ	5.82	1.48	1.37
1	G	437	PHE	CG-CD2	5.61	1.47	1.38
1	A	500	PHE	CG-CD1	5.37	1.46	1.38
1	D	280	TRP	CD2-CE2	5.33	1.47	1.41
1	E	405	GLU	CD-OE2	5.19	1.31	1.25
1	C	41	ARG	CZ-NH1	5.16	1.39	1.33
1	A	368	TRP	CD2-CE2	5.04	1.47	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NE-CZ-NH1	33.04	136.82	120.30
1	F	78	ARG	NE-CZ-NH1	31.73	136.17	120.30
1	C	41	ARG	NE-CZ-NH1	30.25	135.42	120.30
1	H	41	ARG	NE-CZ-NH1	30.19	135.40	120.30
1	H	41	ARG	NE-CZ-NH2	-29.71	105.45	120.30
1	C	41	ARG	NE-CZ-NH2	-28.55	106.03	120.30
1	A	78	ARG	NE-CZ-NH2	-28.14	106.23	120.30
1	F	78	ARG	NE-CZ-NH2	-27.30	106.65	120.30
1	G	41	ARG	NE-CZ-NH2	-13.41	113.60	120.30
1	B	41	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	F	41	ARG	NE-CZ-NH2	-13.03	113.78	120.30
1	B	460	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	D	41	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	E	41	ARG	NE-CZ-NH2	-12.31	114.14	120.30
1	D	41	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	G	41	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	F	78	ARG	CD-NE-CZ	11.52	139.72	123.60
1	B	41	ARG	NE-CZ-NH1	11.45	126.02	120.30
1	A	41	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	F	41	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	A	78	ARG	CD-NE-CZ	11.23	139.32	123.60
1	A	41	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	E	41	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	78	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	460	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	G	460	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	B	460	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	F	460	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	G	78	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	H	460	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	E	78	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	C	460	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	D	78	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	F	302	LEU	CA-CB-CG	8.10	133.94	115.30
1	E	460	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	H	78	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	78	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	460	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	H	460	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	460	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	G	460	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	E	78	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	460	ARG	NE-CZ-NH2	-7.08	116.76	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	F	460	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	C	460	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	510	LYS	CD-CE-NZ	6.68	127.06	111.70
1	H	78	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	F	302	LEU	CB-CG-CD2	6.64	122.30	111.00
1	D	460	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	G	78	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	329	ASP	CB-CA-C	-6.23	97.95	110.40
1	C	78	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	41	ARG	CD-NE-CZ	5.98	131.97	123.60
1	H	144	ASP	CB-CA-C	-5.96	98.49	110.40
1	F	247	LYS	CG-CD-CE	5.91	129.62	111.90
1	D	247	LYS	CG-CD-CE	5.75	129.16	111.90
1	B	331	ASN	N-CA-C	5.74	126.51	111.00
1	H	41	ARG	CD-NE-CZ	5.55	131.37	123.60
1	C	138	ASP	CB-CG-OD1	5.48	123.23	118.30
1	E	299	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	405	GLU	OE1-CD-OE2	-5.24	117.02	123.30
1	B	510	LYS	CG-CD-CE	5.20	127.51	111.90
1	H	470	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	E	405	GLU	CG-CD-OE2	5.18	128.66	118.30
1	F	144	ASP	CB-CA-C	-5.15	100.10	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3712	0	3579	16	0
1	B	3693	0	3562	19	0
1	C	3693	0	3562	26	0
1	D	3712	0	3579	17	0
1	E	3712	0	3579	18	0
1	F	3693	0	3562	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3693	0	3562	21	0
1	H	3712	0	3579	17	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	0	0
2	G	53	0	31	2	0
2	H	53	0	31	0	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	39	0	54	1	0
5	B	39	0	54	2	0
5	C	26	0	36	3	0
5	D	26	0	36	4	0
5	E	39	0	54	4	0
5	F	26	0	36	3	0
5	G	26	0	36	2	0
5	H	26	0	36	0	0
6	A	23	0	22	0	0
6	B	46	0	44	0	0
6	C	23	0	22	0	0
6	D	46	0	43	1	0
6	E	23	0	22	0	0
6	F	46	0	44	0	0
6	G	23	0	22	0	0
6	H	46	0	44	0	0
7	A	473	0	0	3	0
7	B	405	0	0	4	0
7	C	315	0	0	3	0
7	D	321	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	359	0	0	1	0
7	F	296	0	0	2	0
7	G	440	0	0	2	0
7	H	361	0	0	3	0
All	All	33549	0	29417	148	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 (148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:MET:HE1	1:C:349:LEU:HD21	1.25	1.17
1:G:339:MET:HE1	1:G:349:LEU:HD21	1.27	1.15
1:G:339:MET:CE	1:G:349:LEU:HD21	2.04	0.88
1:F:302:LEU:HD13	1:F:432:ILE:HD12	1.62	0.82
1:F:302:LEU:HD22	1:F:340:ILE:HB	1.68	0.76
1:F:302:LEU:HD13	1:F:432:ILE:CD1	2.16	0.76
1:C:339:MET:HE1	1:C:349:LEU:CD2	2.14	0.72
1:C:339:MET:CE	1:C:349:LEU:HD21	2.12	0.71
1:C:249:ILE:HB	7:C:2178:HOH:O	1.89	0.71
1:C:339:MET:CE	1:C:349:LEU:HD11	2.24	0.67
1:B:41:ARG:HD3	7:B:2034:HOH:O	1.96	0.65
5:D:581:PG4:C5	5:D:581:PG4:O1	2.46	0.64
1:A:139:PRO:HG3	5:B:582:PG4:H42	1.80	0.63
1:E:456:ASP:OD2	1:E:460:ARG:HD3	1.99	0.62
1:C:456:ASP:OD2	1:C:460:ARG:HD3	1.99	0.62
1:F:456:ASP:OD2	1:F:460:ARG:HD3	2.00	0.62
1:G:456:ASP:OD2	1:G:460:ARG:HD3	1.99	0.62
1:D:456:ASP:OD2	1:D:460:ARG:HD3	2.00	0.62
1:H:344:ARG:NH1	7:H:2281:HOH:O	2.27	0.61
1:H:456:ASP:OD2	1:H:460:ARG:HD3	2.00	0.61
1:A:456:ASP:OD2	1:A:460:ARG:HD3	2.00	0.61
1:E:139:PRO:HB3	5:F:582:PG4:H42	1.83	0.60
1:A:62:GLU:OE2	1:D:422:ASN:OD1	2.18	0.60
1:E:5:THR:HG21	1:E:217:GLN:HG2	1.85	0.59
1:B:113:PHE:HE2	1:C:65:GLY:HA3	1.67	0.58
1:D:375:GLU:OE2	1:D:389:ARG:NE	2.32	0.58
1:D:344:ARG:NH1	7:D:2238:HOH:O	2.35	0.57
1:B:5:THR:HG21	1:B:217:GLN:HG2	1.86	0.56
1:H:212:SER:OG	1:H:217:GLN:NE2	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:582:PG4:H51	7:B:2405:HOH:O	2.05	0.55
1:A:485:ARG:HD3	7:A:2295:HOH:O	2.06	0.55
1:H:212:SER:HG	1:H:217:GLN:HE22	1.55	0.54
5:D:581:PG4:O1	5:D:581:PG4:H51	2.07	0.53
1:D:5:THR:HG21	1:D:217:GLN:HG2	1.90	0.53
1:E:422:ASN:ND2	1:E:424:GLY:H	2.06	0.53
1:A:441:ARG:NH1	7:A:2421:HOH:O	2.41	0.53
1:G:5:THR:HG21	1:G:217:GLN:HG2	1.90	0.53
1:E:386:ASP:HB3	7:E:2302:HOH:O	2.08	0.53
1:A:5:THR:HG21	1:A:217:GLN:HG2	1.91	0.53
1:F:5:THR:HG21	1:F:217:GLN:HG2	1.91	0.52
1:A:344:ARG:NH1	7:A:2358:HOH:O	2.36	0.51
1:C:5:THR:HG21	1:C:217:GLN:HG2	1.91	0.51
1:H:423:GLY:HA3	7:H:2320:HOH:O	2.10	0.51
1:G:339:MET:CE	1:G:349:LEU:HD11	2.40	0.51
1:B:330:ASP:C	1:B:331:ASN:OD1	2.48	0.51
1:A:375:GLU:OE2	1:A:389:ARG:NE	2.39	0.51
1:A:356:ASN:ND2	1:B:161:ASP:HB3	2.26	0.50
1:G:49:SER:HA	2:G:551:FAD:C6	2.40	0.50
1:D:3:ASP:OD1	1:D:218:ARG:NH1	2.45	0.50
1:F:375:GLU:OE2	1:F:389:ARG:NE	2.36	0.50
1:B:332:GLY:HA2	7:B:2304:HOH:O	2.11	0.50
1:G:339:MET:CE	1:G:349:LEU:CD2	2.84	0.50
1:E:139:PRO:HG3	5:F:582:PG4:H32	1.94	0.50
1:F:386:ASP:HB2	7:F:2256:HOH:O	2.11	0.49
1:G:41:ARG:HD3	7:G:2034:HOH:O	2.12	0.49
1:H:5:THR:HG21	1:H:217:GLN:HG2	1.93	0.49
1:A:422:ASN:ND2	1:D:62:GLU:OE2	2.44	0.49
5:C:582:PG4:H32	1:D:162:HIS:HB2	1.94	0.49
1:C:296:VAL:HG21	5:C:581:PG4:H51	1.94	0.49
1:F:65:GLY:HA3	1:G:113:PHE:HE2	1.78	0.49
1:F:3:ASP:OD1	1:F:218:ARG:NH1	2.45	0.49
1:B:255:PHE:HB2	7:B:2241:HOH:O	2.13	0.49
1:C:87:GLU:HG3	7:C:2060:HOH:O	2.13	0.48
1:G:339:MET:HE1	1:G:349:LEU:CD2	2.19	0.48
1:B:258:ASN:OD1	2:B:551:FAD:H2B	2.14	0.48
1:B:247:LYS:HE2	1:B:250:TRP:CH2	2.49	0.48
1:C:375:GLU:OE2	1:C:389:ARG:NE	2.40	0.48
1:B:329:ASP:CG	1:B:329:ASP:O	2.51	0.48
1:H:247:LYS:HE2	1:H:250:TRP:CH2	2.48	0.48
1:A:52:SER:HB2	5:A:581:PG4:H82	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:SER:HB2	2:G:551:FAD:C4X	2.44	0.47
1:C:339:MET:HE3	1:C:349:LEU:HG	1.97	0.47
5:D:581:PG4:H52	5:D:581:PG4:O1	2.15	0.47
1:G:339:MET:HE3	1:G:349:LEU:CG	2.45	0.47
1:C:382:GLY:HA2	7:C:2264:HOH:O	2.15	0.47
1:C:339:MET:HE3	1:C:349:LEU:CG	2.46	0.46
5:E:581:PG4:O1	5:E:581:PG4:C5	2.64	0.46
1:E:247:LYS:HE2	1:E:250:TRP:CH2	2.51	0.46
1:E:96:ALA:HB3	1:E:97:PRO:HD3	1.98	0.46
1:D:96:ALA:HB3	1:D:97:PRO:HD3	1.98	0.46
1:E:62:GLU:OE2	1:H:422:ASN:OD1	2.34	0.45
1:E:356:ASN:ND2	1:F:161:ASP:HB3	2.32	0.45
1:G:96:ALA:HB3	1:G:97:PRO:HD3	1.98	0.45
1:E:510:LYS:HB2	1:E:510:LYS:HE3	1.62	0.45
1:B:7:GLU:HG2	1:B:220:LYS:HB3	1.98	0.45
1:B:7:GLU:HG2	1:B:220:LYS:HD3	1.99	0.45
5:C:581:PG4:O1	5:C:581:PG4:O3	2.35	0.45
1:G:247:LYS:HE2	1:G:250:TRP:CH2	2.51	0.45
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.99	0.45
1:D:49:SER:HA	2:D:551:FAD:C6	2.47	0.44
1:E:477:ASN:ND2	2:E:551:FAD:H5'2	2.31	0.44
5:G:582:PG4:H11	1:H:164:PRO:HA	1.98	0.44
1:C:435:GLY:HA2	1:C:436:PRO:C	2.38	0.44
1:A:435:GLY:HA2	1:A:436:PRO:C	2.38	0.44
1:G:375:GLU:OE2	1:G:389:ARG:NE	2.39	0.44
1:H:96:ALA:HB3	1:H:97:PRO:HD3	1.99	0.44
1:C:247:LYS:HE2	1:C:250:TRP:CH2	2.52	0.44
1:C:161:ASP:HB3	1:D:356:ASN:ND2	2.32	0.44
1:F:96:ALA:HB3	1:F:97:PRO:HD3	1.99	0.44
1:A:96:ALA:HB3	1:A:97:PRO:HD3	1.98	0.44
1:E:164:PRO:HG3	7:F:2120:HOH:O	2.16	0.44
1:G:161:ASP:HB3	1:H:356:ASN:ND2	2.32	0.43
1:D:52:SER:HB2	5:D:581:PG4:H82	2.00	0.43
1:B:482:LEU:HD12	1:B:482:LEU:C	2.39	0.43
1:G:339:MET:HE3	1:G:349:LEU:HG	2.00	0.43
1:C:339:MET:CE	1:C:349:LEU:CG	2.97	0.43
1:H:211:GLU:OE2	1:H:216:THR:HB	2.19	0.43
1:E:211:GLU:OE2	1:E:216:THR:HB	2.19	0.43
1:F:211:GLU:OE2	1:F:216:THR:HB	2.19	0.42
1:D:211:GLU:OE2	1:D:216:THR:HB	2.20	0.42
1:B:211:GLU:OE2	1:B:216:THR:HB	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:SER:HA	2:C:551:FAD:C6	2.49	0.42
6:D:592:SUC:H6'1	6:D:592:SUC:O5	2.19	0.42
1:E:49:SER:HB2	2:E:551:FAD:C4X	2.49	0.42
1:A:211:GLU:OE2	1:A:216:THR:HB	2.19	0.42
1:C:96:ALA:HB3	1:C:97:PRO:HD3	2.01	0.42
1:D:49:SER:HB2	2:D:551:FAD:C4X	2.49	0.42
1:G:211:GLU:OE2	1:G:216:THR:HB	2.20	0.42
5:G:582:PG4:C1	1:H:164:PRO:HA	2.50	0.42
1:A:247:LYS:HE2	1:A:250:TRP:CH2	2.54	0.42
1:C:211:GLU:OE2	1:C:216:THR:HB	2.20	0.42
1:H:435:GLY:HA2	1:H:436:PRO:C	2.40	0.42
1:C:59:GLN:O	1:C:63:ARG:HG3	2.20	0.41
1:C:356:ASN:ND2	1:D:161:ASP:HB3	2.35	0.41
1:F:59:GLN:O	1:F:63:ARG:HG3	2.20	0.41
1:G:249:ILE:HB	7:G:2245:HOH:O	2.20	0.41
1:A:59:GLN:O	1:A:63:ARG:HG3	2.21	0.41
1:G:59:GLN:O	1:G:63:ARG:HG3	2.20	0.41
1:H:456:ASP:HB2	7:H:2329:HOH:O	2.20	0.41
1:C:339:MET:HE2	1:C:349:LEU:HD11	2.03	0.41
1:H:59:GLN:O	1:H:63:ARG:HG3	2.20	0.41
1:D:477:ASN:ND2	2:D:551:FAD:H5'2	2.36	0.41
1:F:482:LEU:C	1:F:482:LEU:HD12	2.41	0.41
1:B:331:ASN:HB2	1:B:333:SER:HB3	2.03	0.41
1:C:339:MET:CE	1:C:349:LEU:CD2	2.88	0.41
1:E:52:SER:HB2	5:E:581:PG4:H81	2.01	0.41
1:H:422:ASN:C	1:H:423:GLY:O	2.58	0.41
1:B:284:GLY:HA2	1:B:293:ALA:O	2.22	0.40
1:E:375:GLU:OE2	1:E:389:ARG:NE	2.40	0.40
5:E:581:PG4:H51	5:E:581:PG4:O1	2.21	0.40
1:E:139:PRO:CB	5:F:582:PG4:H42	2.51	0.40
1:B:59:GLN:O	1:B:63:ARG:HG3	2.20	0.40
5:E:581:PG4:O1	5:E:581:PG4:H52	2.21	0.40
1:G:435:GLY:HA2	1:G:436:PRO:C	2.42	0.40
1:D:297:GLY:HA2	1:D:418:PHE:CG	2.57	0.40
1:B:330:ASP:O	1:B:331:ASN:OD1	2.39	0.40
1:C:284:GLY:HA2	1:C:293:ALA:O	2.21	0.40
1:F:284:GLY:HA2	1:F:293:ALA:O	2.21	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%)	493 (97%)	12 (2%)	1 (0%)	51	48
1	B	501/530 (94%)	487 (97%)	14 (3%)	0	100	100
1	C	501/530 (94%)	489 (98%)	12 (2%)	0	100	100
1	D	506/530 (96%)	493 (97%)	12 (2%)	1 (0%)	51	48
1	E	506/530 (96%)	494 (98%)	11 (2%)	1 (0%)	51	48
1	F	501/530 (94%)	489 (98%)	12 (2%)	0	100	100
1	G	501/530 (94%)	490 (98%)	11 (2%)	0	100	100
1	H	506/530 (96%)	495 (98%)	10 (2%)	1 (0%)	51	48
All	All	4028/4240 (95%)	3930 (98%)	94 (2%)	4 (0%)	55	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	GLY
1	H	423	GLY
1	D	423	GLY
1	E	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%)	361 (98%)	8 (2%)	57	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	367/388 (95%)	359 (98%)	8 (2%)	57	60
1	C	367/388 (95%)	361 (98%)	6 (2%)	68	72
1	D	369/388 (95%)	359 (97%)	10 (3%)	50	51
1	E	369/388 (95%)	361 (98%)	8 (2%)	57	60
1	F	367/388 (95%)	358 (98%)	9 (2%)	53	54
1	G	367/388 (95%)	360 (98%)	7 (2%)	62	66
1	H	369/388 (95%)	362 (98%)	7 (2%)	62	66
All	All	2944/3104 (95%)	2881 (98%)	63 (2%)	59	62

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	158	THR
1	A	171	ARG
1	A	216	THR
1	A	312	LEU
1	A	318	TYR
1	A	485	ARG
1	A	487	TYR
1	B	78	ARG
1	B	158	THR
1	B	171	ARG
1	B	216	THR
1	B	237	GLU
1	B	312	LEU
1	B	318	TYR
1	B	487	TYR
1	C	158	THR
1	C	171	ARG
1	C	216	THR
1	C	312	LEU
1	C	485	ARG
1	C	487	TYR
1	D	105	GLN
1	D	158	THR
1	D	171	ARG
1	D	216	THR
1	D	237	GLU
1	D	241	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	312	LEU
1	D	389	ARG
1	D	485	ARG
1	D	487	TYR
1	E	158	THR
1	E	171	ARG
1	E	216	THR
1	E	312	LEU
1	E	422	ASN
1	E	485	ARG
1	E	487	TYR
1	E	510	LYS
1	F	78	ARG
1	F	158	THR
1	F	171	ARG
1	F	216	THR
1	F	237	GLU
1	F	302	LEU
1	F	312	LEU
1	F	485	ARG
1	F	487	TYR
1	G	158	THR
1	G	171	ARG
1	G	216	THR
1	G	312	LEU
1	G	318	TYR
1	G	485	ARG
1	G	487	TYR
1	H	158	THR
1	H	171	ARG
1	H	216	THR
1	H	312	LEU
1	H	386	ASP
1	H	485	ARG
1	H	487	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	217	GLN
1	D	422	ASN
1	E	217	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	422	ASN
1	H	217	GLN
1	H	241	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 12 are monoatomic - leaving 39 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	-	51,58,58	2.21	11 (21%)	54,89,89	2.54	16 (29%)
5	PG4	A	581	-	12,12,12	0.99	0	11,11,11	0.76	0
5	PG4	A	582	-	12,12,12	0.91	0	11,11,11	0.64	0
5	PG4	A	583	-	12,12,12	0.99	0	11,11,11	1.31	1 (9%)
6	SUC	A	591	-	24,24,24	1.18	3 (12%)	36,36,36	0.99	2 (5%)
2	FAD	B	551	-	51,58,58	1.80	10 (19%)	54,89,89	2.47	9 (16%)
5	PG4	B	581	-	12,12,12	0.68	0	11,11,11	0.59	0
5	PG4	B	582	-	12,12,12	0.92	0	11,11,11	0.79	0
5	PG4	B	584	-	12,12,12	0.81	0	11,11,11	1.16	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SUC	B	591	-	24,24,24	1.36	3 (12%)	36,36,36	1.58	8 (22%)
6	SUC	B	592	-	24,24,24	1.73	8 (33%)	36,36,36	0.87	1 (2%)
2	FAD	C	551	-	51,58,58	1.96	11 (21%)	54,89,89	2.17	9 (16%)
5	PG4	C	581	-	12,12,12	0.94	0	11,11,11	1.23	1 (9%)
5	PG4	C	582	-	12,12,12	0.88	0	11,11,11	0.89	0
6	SUC	C	591	-	24,24,24	1.17	2 (8%)	36,36,36	0.96	1 (2%)
2	FAD	D	551	-	51,58,58	2.05	11 (21%)	54,89,89	2.50	9 (16%)
5	PG4	D	581	-	12,12,12	0.96	0	11,11,11	0.64	0
5	PG4	D	582	-	12,12,12	0.94	0	11,11,11	0.64	0
6	SUC	D	591	-	24,24,24	1.32	4 (16%)	36,36,36	0.98	2 (5%)
6	SUC	D	592	-	24,24,24	1.35	4 (16%)	36,36,36	1.34	1 (2%)
2	FAD	E	551	-	51,58,58	1.72	8 (15%)	54,89,89	2.57	15 (27%)
5	PG4	E	581	-	12,12,12	0.87	0	11,11,11	0.52	0
5	PG4	E	582	-	12,12,12	1.03	0	11,11,11	0.95	0
5	PG4	E	583	-	12,12,12	1.00	0	11,11,11	1.20	1 (9%)
6	SUC	E	591	-	24,24,24	1.20	4 (16%)	36,36,36	0.91	0
2	FAD	F	551	-	51,58,58	1.70	7 (13%)	54,89,89	2.33	11 (20%)
5	PG4	F	581	-	12,12,12	0.99	1 (8%)	11,11,11	0.51	0
5	PG4	F	582	-	12,12,12	0.91	0	11,11,11	1.07	1 (9%)
6	SUC	F	591	-	24,24,24	1.65	6 (25%)	36,36,36	1.49	6 (16%)
6	SUC	F	592	-	24,24,24	1.52	4 (16%)	36,36,36	1.18	2 (5%)
2	FAD	G	551	-	51,58,58	1.93	13 (25%)	54,89,89	2.19	10 (18%)
5	PG4	G	581	-	12,12,12	0.75	0	11,11,11	0.59	0
5	PG4	G	582	-	12,12,12	0.87	0	11,11,11	0.64	0
6	SUC	G	591	-	24,24,24	1.11	2 (8%)	36,36,36	1.05	2 (5%)
2	FAD	H	551	-	51,58,58	1.81	9 (17%)	54,89,89	2.43	11 (20%)
5	PG4	H	581	-	12,12,12	0.85	0	11,11,11	0.70	0
5	PG4	H	582	-	12,12,12	0.77	0	11,11,11	0.82	0
6	SUC	H	591	-	24,24,24	1.13	2 (8%)	36,36,36	1.11	4 (11%)
6	SUC	H	592	-	24,24,24	1.55	5 (20%)	36,36,36	1.02	1 (2%)

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	-	-	0/28/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	A	581	-	-	0/10/10/10	0/0/0/0
5	PG4	A	582	-	-	0/10/10/10	0/0/0/0
5	PG4	A	583	-	-	0/10/10/10	0/0/0/0
6	SUC	A	591	-	-	0/12/51/51	0/2/2/2
2	FAD	B	551	-	-	0/28/50/50	0/6/6/6
5	PG4	B	581	-	-	0/10/10/10	0/0/0/0
5	PG4	B	582	-	-	0/10/10/10	0/0/0/0
5	PG4	B	584	-	-	0/10/10/10	0/0/0/0
6	SUC	B	591	-	-	0/12/51/51	0/2/2/2
6	SUC	B	592	-	-	0/12/51/51	0/2/2/2
2	FAD	C	551	-	-	0/28/50/50	0/6/6/6
5	PG4	C	581	-	-	0/10/10/10	0/0/0/0
5	PG4	C	582	-	-	0/10/10/10	0/0/0/0
6	SUC	C	591	-	-	0/12/51/51	0/2/2/2
2	FAD	D	551	-	-	0/28/50/50	0/6/6/6
5	PG4	D	581	-	-	0/10/10/10	0/0/0/0
5	PG4	D	582	-	-	0/10/10/10	0/0/0/0
6	SUC	D	591	-	-	0/12/51/51	0/2/2/2
6	SUC	D	592	-	-	0/12/51/51	0/2/2/2
2	FAD	E	551	-	-	0/28/50/50	0/6/6/6
5	PG4	E	581	-	-	0/10/10/10	0/0/0/0
5	PG4	E	582	-	-	0/10/10/10	0/0/0/0
5	PG4	E	583	-	-	0/10/10/10	0/0/0/0
6	SUC	E	591	-	-	0/12/51/51	0/2/2/2
2	FAD	F	551	-	-	0/28/50/50	0/6/6/6
5	PG4	F	581	-	-	0/10/10/10	0/0/0/0
5	PG4	F	582	-	-	0/10/10/10	0/0/0/0
6	SUC	F	591	-	-	0/12/51/51	0/2/2/2
6	SUC	F	592	-	-	0/12/51/51	0/2/2/2
2	FAD	G	551	-	-	0/28/50/50	0/6/6/6
5	PG4	G	581	-	-	0/10/10/10	0/0/0/0
5	PG4	G	582	-	-	0/10/10/10	0/0/0/0
6	SUC	G	591	-	-	0/12/51/51	0/2/2/2
2	FAD	H	551	-	-	0/28/50/50	0/6/6/6
5	PG4	H	581	-	-	0/10/10/10	0/0/0/0
5	PG4	H	582	-	-	0/10/10/10	0/0/0/0
6	SUC	H	591	-	-	0/12/51/51	0/2/2/2
6	SUC	H	592	-	-	0/12/51/51	0/2/2/2

All (128) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	551	FAD	C7M-C7	-5.83	1.39	1.51
2	E	551	FAD	C7M-C7	-5.61	1.40	1.51
2	G	551	FAD	C8M-C8	-5.51	1.40	1.51
2	F	551	FAD	C8M-C8	-5.50	1.40	1.51
2	D	551	FAD	C7M-C7	-5.48	1.40	1.51
2	A	551	FAD	C8M-C8	-5.08	1.41	1.51
2	C	551	FAD	C8M-C8	-4.97	1.41	1.51
2	H	551	FAD	C7M-C7	-4.91	1.41	1.51
2	A	551	FAD	C7M-C7	-4.52	1.42	1.51
2	E	551	FAD	C8M-C8	-4.51	1.42	1.51
2	G	551	FAD	C7M-C7	-4.49	1.42	1.51
2	F	551	FAD	C7M-C7	-4.47	1.42	1.51
2	B	551	FAD	C7M-C7	-4.38	1.42	1.51
2	D	551	FAD	C8M-C8	-4.33	1.42	1.51
2	B	551	FAD	C8M-C8	-4.16	1.42	1.51
2	H	551	FAD	C5A-C4A	-3.68	1.32	1.40
2	H	551	FAD	C8M-C8	-3.51	1.44	1.51
2	A	551	FAD	C5A-C4A	-3.32	1.33	1.40
2	F	551	FAD	C5A-C4A	-2.79	1.34	1.40
6	D	591	SUC	O2-C2	-2.68	1.36	1.43
2	G	551	FAD	C9A-N10	-2.61	1.35	1.38
2	D	551	FAD	C5A-C4A	-2.59	1.34	1.40
2	E	551	FAD	C5A-C4A	-2.49	1.34	1.40
2	B	551	FAD	C4'-C3'	-2.33	1.48	1.53
2	F	551	FAD	P-O2P	-2.28	1.43	1.55
6	A	591	SUC	O3'-C3'	-2.26	1.38	1.42
2	H	551	FAD	C2-N1	-2.24	1.33	1.38
2	B	551	FAD	C5A-C4A	-2.21	1.35	1.40
2	A	551	FAD	C4'-C3'	-2.19	1.49	1.53
2	G	551	FAD	C5A-N7A	-2.15	1.32	1.39
6	A	591	SUC	O2-C2	-2.14	1.38	1.43
2	C	551	FAD	C6-C5X	-2.11	1.38	1.41
2	E	551	FAD	C4'-C3'	-2.10	1.49	1.53
6	G	591	SUC	O4'-C4'	2.02	1.47	1.43
6	B	592	SUC	C3-C2	2.02	1.57	1.52
2	G	551	FAD	C2'-C3'	2.05	1.57	1.53
6	D	591	SUC	O5-C5	2.05	1.49	1.44
6	F	591	SUC	O4'-C4'	2.05	1.47	1.43
5	F	581	PG4	O2-C2	2.06	1.50	1.42
2	G	551	FAD	C4X-N5	2.07	1.36	1.33
6	G	591	SUC	O4-C4	2.07	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	591	SUC	O4'-C4'	2.11	1.47	1.43
6	D	592	SUC	O3-C3	2.12	1.47	1.43
6	F	591	SUC	O4-C4	2.14	1.47	1.43
2	A	551	FAD	O4B-C1B	2.18	1.44	1.41
2	D	551	FAD	C2B-C1B	2.19	1.57	1.53
6	B	592	SUC	O1-C2'	2.20	1.52	1.43
2	H	551	FAD	C10-N1	2.23	1.36	1.33
2	G	551	FAD	C2-N1	2.24	1.42	1.38
2	B	551	FAD	C1'-N10	2.25	1.50	1.48
6	D	592	SUC	C4-C5	2.30	1.57	1.53
6	B	591	SUC	C4-C3	2.30	1.58	1.52
2	C	551	FAD	O4B-C4B	2.33	1.50	1.45
6	H	591	SUC	O2'-C5'	2.33	1.49	1.43
6	A	591	SUC	O5-C1	2.33	1.47	1.41
6	B	592	SUC	O4-C4	2.35	1.48	1.43
2	D	551	FAD	O4B-C1B	2.36	1.44	1.41
2	C	551	FAD	O3B-C3B	2.36	1.48	1.43
6	F	591	SUC	C4-C3	2.39	1.58	1.52
6	D	591	SUC	O2'-C2'	2.40	1.48	1.42
6	E	591	SUC	O5-C5	2.40	1.50	1.44
6	H	592	SUC	C4-C3	2.40	1.58	1.52
6	B	592	SUC	O5-C1	2.40	1.47	1.41
6	B	592	SUC	C4-C5	2.42	1.58	1.53
6	E	591	SUC	O2'-C5'	2.50	1.49	1.43
2	B	551	FAD	C10-N1	2.53	1.36	1.33
6	D	592	SUC	O2-C2	2.57	1.48	1.43
6	D	591	SUC	O2'-C5'	2.58	1.49	1.43
6	D	592	SUC	O5-C5	2.60	1.50	1.44
6	B	592	SUC	O3-C3	2.66	1.49	1.43
2	E	551	FAD	C10-N1	2.69	1.37	1.33
6	C	591	SUC	C4'-C5'	2.70	1.60	1.53
6	E	591	SUC	O4-C4	2.74	1.49	1.43
6	F	591	SUC	O5-C1	2.76	1.48	1.41
6	C	591	SUC	O2'-C2'	2.76	1.48	1.42
6	F	592	SUC	C4-C3	2.77	1.59	1.52
6	H	592	SUC	O3-C3	2.79	1.49	1.43
2	D	551	FAD	O4B-C4B	2.83	1.51	1.45
6	H	591	SUC	O2'-C2'	2.87	1.49	1.42
6	B	591	SUC	O2'-C2'	2.88	1.49	1.42
2	C	551	FAD	O4B-C1B	2.89	1.45	1.41
6	H	592	SUC	O2'-C2'	2.94	1.49	1.42
6	B	592	SUC	O2-C2	2.95	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	551	FAD	C10-N1	2.97	1.37	1.33
2	A	551	FAD	C10-N1	2.97	1.37	1.33
2	C	551	FAD	C10-N1	3.00	1.37	1.33
6	F	591	SUC	O2'-C5'	3.02	1.50	1.43
6	H	592	SUC	O2-C2	3.06	1.50	1.43
2	C	551	FAD	C1'-N10	3.08	1.51	1.48
6	F	592	SUC	O2'-C2'	3.08	1.49	1.42
2	D	551	FAD	C2A-N1A	3.13	1.39	1.33
2	G	551	FAD	C2B-C1B	3.14	1.58	1.53
2	G	551	FAD	C4-N3	3.16	1.38	1.33
2	C	551	FAD	C4-N3	3.16	1.38	1.33
6	F	592	SUC	O5-C5	3.18	1.52	1.44
6	H	592	SUC	O5-C1	3.23	1.49	1.41
2	A	551	FAD	C4X-N5	3.23	1.38	1.33
2	E	551	FAD	C2A-N1A	3.34	1.40	1.33
2	B	551	FAD	C5'-C4'	3.36	1.56	1.51
2	H	551	FAD	C4-N3	3.36	1.39	1.33
6	B	591	SUC	O2'-C5'	3.43	1.51	1.43
2	D	551	FAD	C4-N3	3.45	1.39	1.33
2	G	551	FAD	C2A-N1A	3.46	1.40	1.33
2	B	551	FAD	C4-N3	3.48	1.39	1.33
2	A	551	FAD	C2A-N1A	3.49	1.40	1.33
2	H	551	FAD	C2B-C1B	3.50	1.59	1.53
2	G	551	FAD	C2A-N3A	3.54	1.38	1.32
2	F	551	FAD	C4-N3	3.55	1.39	1.33
6	B	592	SUC	O2'-C2'	3.60	1.50	1.42
2	F	551	FAD	C2A-N3A	3.68	1.38	1.32
6	F	592	SUC	O2-C2	3.68	1.51	1.43
2	D	551	FAD	C10-N1	3.77	1.38	1.33
2	A	551	FAD	C4-N3	3.82	1.40	1.33
2	B	551	FAD	C2A-N3A	3.84	1.38	1.32
2	D	551	FAD	C1'-N10	3.95	1.52	1.48
2	C	551	FAD	C2A-N1A	3.95	1.41	1.33
2	E	551	FAD	C4-N3	4.10	1.40	1.33
6	F	591	SUC	O2'-C2'	4.29	1.52	1.42
2	H	551	FAD	C2A-N3A	4.33	1.39	1.32
2	B	551	FAD	C2A-N1A	4.46	1.42	1.33
2	F	551	FAD	C10-N1	4.66	1.39	1.33
2	H	551	FAD	C1'-N10	4.75	1.53	1.48
2	E	551	FAD	C2A-N3A	4.80	1.40	1.32
2	G	551	FAD	C1'-N10	5.61	1.54	1.48
2	A	551	FAD	C2A-N3A	6.01	1.42	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	551	FAD	C2A-N3A	6.19	1.42	1.32
2	D	551	FAD	C2A-N3A	6.84	1.43	1.32
2	A	551	FAD	C1'-N10	7.86	1.56	1.48

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	551	FAD	N3A-C2A-N1A	-13.06	117.48	128.86
2	E	551	FAD	N3A-C2A-N1A	-12.70	117.79	128.86
2	B	551	FAD	N3A-C2A-N1A	-12.45	118.01	128.86
2	D	551	FAD	N3A-C2A-N1A	-12.17	118.26	128.86
2	A	551	FAD	N3A-C2A-N1A	-12.00	118.41	128.86
2	F	551	FAD	N3A-C2A-N1A	-10.32	119.87	128.86
2	G	551	FAD	N3A-C2A-N1A	-9.90	120.23	128.86
2	C	551	FAD	N3A-C2A-N1A	-9.70	120.41	128.86
2	G	551	FAD	C4'-C3'-C2'	-4.57	103.58	113.41
2	E	551	FAD	C4B-O4B-C1B	-4.48	105.00	109.77
6	B	591	SUC	C6'-C5'-C4'	-4.28	104.71	115.05
2	D	551	FAD	C4B-O4B-C1B	-4.25	105.24	109.77
2	F	551	FAD	C4B-O4B-C1B	-4.25	105.25	109.77
2	E	551	FAD	C1B-N9A-C4A	-4.21	119.36	126.64
2	H	551	FAD	C1B-N9A-C4A	-4.15	119.47	126.64
6	F	591	SUC	O1-C2'-C1'	-4.02	96.58	109.51
2	C	551	FAD	C4B-O4B-C1B	-4.00	105.52	109.77
2	C	551	FAD	C4'-C3'-C2'	-3.92	104.98	113.41
2	B	551	FAD	C4'-C3'-C2'	-3.68	105.50	113.41
2	A	551	FAD	C1B-N9A-C4A	-3.59	120.43	126.64
2	F	551	FAD	C4'-C3'-C2'	-3.57	105.72	113.41
2	F	551	FAD	C1B-N9A-C4A	-3.54	120.52	126.64
2	B	551	FAD	C4X-C4-N3	-3.51	118.48	123.48
2	G	551	FAD	C10-C4X-N5	-3.45	116.62	120.59
2	D	551	FAD	C1B-N9A-C4A	-3.39	120.78	126.64
2	D	551	FAD	C4X-C4-N3	-3.35	118.72	123.48
2	B	551	FAD	C1B-N9A-C4A	-3.31	120.92	126.64
2	E	551	FAD	C4'-C3'-C2'	-3.18	106.56	113.41
2	E	551	FAD	C4X-C4-N3	-3.17	118.97	123.48
6	F	592	SUC	C2'-O1-C1	-3.08	109.38	117.62
2	D	551	FAD	C4'-C3'-C2'	-3.06	106.83	113.41
2	A	551	FAD	C4'-C3'-C2'	-3.03	106.88	113.41
2	F	551	FAD	C4X-C4-N3	-2.89	119.36	123.48
6	B	591	SUC	O1-C2'-C1'	-2.89	100.21	109.51
2	H	551	FAD	C4'-C3'-C2'	-2.89	107.20	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	551	FAD	C4X-C4-N3	-2.85	119.43	123.48
6	G	591	SUC	O2-C2-C1	-2.74	104.31	110.03
2	A	551	FAD	C4B-O4B-C1B	-2.61	106.99	109.77
6	B	591	SUC	C6-C5-C4	-2.59	106.94	113.00
2	A	551	FAD	C4-C4X-C10	-2.56	117.89	119.96
6	A	591	SUC	C2'-O1-C1	-2.54	110.82	117.62
2	C	551	FAD	C4X-C4-N3	-2.43	120.02	123.48
2	C	551	FAD	C4A-C5A-N7A	-2.43	107.06	109.41
2	A	551	FAD	O4B-C4B-C5B	-2.40	101.31	109.40
2	G	551	FAD	C4B-O4B-C1B	-2.40	107.22	109.77
2	A	551	FAD	C4X-C4-N3	-2.38	120.09	123.48
6	D	591	SUC	O6'-C6'-C5'	-2.36	103.41	111.34
2	G	551	FAD	C4X-C4-N3	-2.31	120.20	123.48
6	F	591	SUC	C6-C5-C4	-2.31	107.60	113.00
2	E	551	FAD	C4A-C5A-N7A	-2.25	107.23	109.41
6	H	591	SUC	C2'-O1-C1	-2.24	111.64	117.62
6	C	591	SUC	O2'-C5'-C6'	-2.19	102.38	108.71
2	A	551	FAD	C4A-C5A-N7A	-2.18	107.30	109.41
2	A	551	FAD	C5A-C6A-N6A	-2.18	116.02	120.47
6	G	591	SUC	C2'-O1-C1	-2.17	111.82	117.62
2	B	551	FAD	C4A-C5A-N7A	-2.12	107.36	109.41
2	F	551	FAD	C4A-C5A-N7A	-2.12	107.36	109.41
6	H	591	SUC	C6'-C5'-C4'	-2.11	109.94	115.05
2	H	551	FAD	O3B-C3B-C4B	-2.09	104.98	111.09
6	H	591	SUC	O6'-C6'-C5'	-2.05	104.43	111.34
6	H	591	SUC	C6-C5-C4	-2.03	108.25	113.00
2	A	551	FAD	C9A-C5X-N5	-2.01	119.24	122.24
2	E	551	FAD	O5'-P-O1P	-2.01	101.14	109.25
6	B	591	SUC	O1-C2'-O2'	2.03	116.79	110.55
2	E	551	FAD	O3'-C3'-C2'	2.08	113.96	108.82
2	E	551	FAD	C1'-C2'-C3'	2.08	115.78	109.82
2	E	551	FAD	C4-C4X-N5	2.13	121.02	118.68
2	F	551	FAD	C4-C4X-N5	2.16	121.05	118.68
5	F	582	PG4	C3-O2-C2	2.16	122.68	113.30
2	H	551	FAD	O2P-P-O1P	2.19	123.62	112.28
5	C	581	PG4	C3-O2-C2	2.24	123.00	113.30
2	A	551	FAD	O2P-P-O1P	2.27	124.04	112.28
5	E	583	PG4	C3-O2-C2	2.30	123.27	113.30
6	D	591	SUC	O2'-C5'-C6'	2.31	115.38	108.71
6	F	591	SUC	C1-O5-C5	2.31	118.07	113.72
2	H	551	FAD	C4-C4X-N5	2.35	121.26	118.68
6	A	591	SUC	O2'-C2'-C1'	2.39	114.23	108.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	591	SUC	O4-C4-C3	2.40	115.58	110.36
6	H	592	SUC	O1-C2'-O2'	2.42	117.99	110.55
2	H	551	FAD	C5X-C9A-N10	2.43	119.46	117.66
2	A	551	FAD	C4X-N5-C5X	2.44	119.34	116.76
6	B	591	SUC	C1-O5-C5	2.47	118.36	113.72
6	B	591	SUC	O2'-C5'-C6'	2.47	115.86	108.71
6	F	592	SUC	O5-C5-C6	2.55	112.51	106.41
2	D	551	FAD	O2P-P-O1P	2.57	125.57	112.28
6	B	591	SUC	O2'-C2'-C1'	2.57	114.69	108.03
6	F	591	SUC	O4-C4-C3	2.58	115.98	110.36
2	F	551	FAD	O3'-C3'-C2'	2.61	115.28	108.82
2	H	551	FAD	C1'-N10-C10	2.64	121.21	118.50
6	F	591	SUC	O2'-C5'-C6'	2.64	116.36	108.71
2	E	551	FAD	C6-C5X-C9A	2.65	122.44	119.00
2	B	551	FAD	C4-C4X-N5	2.68	121.61	118.68
5	B	584	PG4	C5-O3-C4	2.73	125.14	113.30
2	C	551	FAD	C4-C4X-N5	2.76	121.70	118.68
2	A	551	FAD	C5X-C9A-N10	2.79	119.73	117.66
2	D	551	FAD	C4X-C10-N10	2.82	122.48	120.52
2	G	551	FAD	C4X-C10-N10	2.86	122.50	120.52
2	E	551	FAD	C4X-N5-C5X	2.88	119.80	116.76
5	A	583	PG4	C3-O2-C2	2.97	126.16	113.30
2	C	551	FAD	C4X-N5-C5X	3.05	119.98	116.76
2	A	551	FAD	O2'-C2'-C1'	3.10	116.95	109.79
2	F	551	FAD	C5X-C9A-N10	3.14	119.99	117.66
2	B	551	FAD	C4X-N5-C5X	3.24	120.19	116.76
6	B	592	SUC	O5-C5-C6	3.26	114.22	106.41
2	H	551	FAD	C1'-N10-C9A	3.29	121.36	118.35
6	F	591	SUC	O2'-C2'-C1'	3.49	117.08	108.03
2	E	551	FAD	C5X-C9A-N10	3.59	120.32	117.66
2	A	551	FAD	C4-C4X-N5	3.75	122.79	118.68
2	G	551	FAD	C4X-N5-C5X	3.88	120.86	116.76
2	B	551	FAD	C1'-N10-C9A	3.93	121.95	118.35
2	E	551	FAD	C1'-N10-C9A	3.95	121.97	118.35
2	G	551	FAD	C4-C4X-N5	4.11	123.19	118.68
2	G	551	FAD	C1'-N10-C9A	4.41	122.39	118.35
2	F	551	FAD	C1'-N10-C9A	4.45	122.42	118.35
2	G	551	FAD	C4-N3-C2	4.70	119.27	115.16
2	C	551	FAD	C1'-N10-C9A	4.95	122.88	118.35
2	D	551	FAD	C1'-N10-C9A	4.95	122.88	118.35
6	D	592	SUC	O5-C5-C6	5.06	118.53	106.41
2	C	551	FAD	C4-N3-C2	5.29	119.79	115.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	551	FAD	C4-N3-C2	6.20	120.58	115.16
2	E	551	FAD	C4-N3-C2	6.48	120.83	115.16
2	F	551	FAD	C4-N3-C2	7.11	121.38	115.16
2	D	551	FAD	C4-N3-C2	7.36	121.59	115.16
2	B	551	FAD	C4-N3-C2	7.51	121.73	115.16
2	A	551	FAD	C4-N3-C2	7.59	121.80	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	581	PG4	1	0
2	B	551	FAD	1	0
5	B	582	PG4	2	0
2	C	551	FAD	1	0
5	C	581	PG4	2	0
5	C	582	PG4	1	0
2	D	551	FAD	3	0
5	D	581	PG4	4	0
6	D	592	SUC	1	0
2	E	551	FAD	2	0
5	E	581	PG4	4	0
5	F	582	PG4	3	0
2	G	551	FAD	2	0
5	G	582	PG4	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	508/530 (95%)	-0.07	9 (1%) 69 68	19, 26, 43, 74	0
1	B	505/530 (95%)	-0.15	9 (1%) 69 68	19, 28, 47, 67	0
1	C	505/530 (95%)	0.07	18 (3%) 43 44	21, 33, 52, 81	0
1	D	508/530 (95%)	0.09	15 (2%) 51 51	21, 32, 52, 77	0
1	E	508/530 (95%)	-0.01	15 (2%) 51 51	19, 30, 51, 77	0
1	F	505/530 (95%)	0.04	19 (3%) 41 41	18, 33, 53, 84	0
1	G	505/530 (95%)	-0.16	7 (1%) 75 75	18, 27, 44, 68	0
1	H	508/530 (95%)	0.02	16 (3%) 49 49	20, 28, 49, 96	0
All	All	4052/4240 (95%)	-0.02	108 (2%) 55 54	18, 30, 50, 96	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	214	GLY	7.3
1	H	331	ASN	5.6
1	C	420	PRO	5.3
1	A	213	GLY	5.1
1	E	3	ASP	4.6
1	H	213	GLY	4.6
1	G	213	GLY	4.6
1	F	332	GLY	4.5
1	F	331	ASN	4.1
1	D	202	ASP	4.1
1	C	213	GLY	4.0
1	C	3	ASP	4.0
1	B	375	GLU	3.8
1	E	4	TRP	3.7
1	C	400	LYS	3.7
1	E	5	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	214	GLY	3.6
1	F	215	GLU	3.6
1	E	401	LEU	3.5
1	C	4	TRP	3.5
1	C	424	GLY	3.5
1	D	215	GLU	3.4
1	F	420	PRO	3.4
1	G	420	PRO	3.4
1	G	3	ASP	3.3
1	G	214	GLY	3.3
1	F	424	GLY	3.3
1	E	215	GLU	3.2
1	H	389	ARG	3.2
1	F	3	ASP	3.2
1	H	400	LYS	3.1
1	A	3	ASP	3.1
1	C	215	GLU	3.1
1	C	434	ASN	3.0
1	D	400	LYS	3.0
1	C	401	LEU	3.0
1	F	386	ASP	3.0
1	F	425	ALA	3.0
1	H	214	GLY	3.0
1	D	389	ARG	3.0
1	E	202	ASP	3.0
1	H	3	ASP	3.0
1	D	401	LEU	3.0
1	A	215	GLU	2.9
1	C	425	ALA	2.9
1	B	425	ALA	2.9
1	B	215	GLU	2.9
1	B	330	ASP	2.8
1	A	422	ASN	2.8
1	D	465	ASP	2.8
1	H	215	GLU	2.8
1	D	331	ASN	2.8
1	E	213	GLY	2.7
1	B	332	GLY	2.7
1	G	215	GLU	2.7
1	H	434	ASN	2.7
1	H	332	GLY	2.7
1	D	466	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	399	ALA	2.7
1	D	84	ALA	2.6
1	H	387	ALA	2.6
1	A	401	LEU	2.6
1	E	216	THR	2.6
1	D	397	ASP	2.6
1	F	307	ALA	2.6
1	B	213	GLY	2.6
1	H	401	LEU	2.6
1	F	4	TRP	2.5
1	D	3	ASP	2.5
1	H	4	TRP	2.5
1	E	400	LYS	2.5
1	E	7	GLU	2.5
1	A	214	GLY	2.4
1	G	425	ALA	2.4
1	G	212	SER	2.4
1	F	212	SER	2.3
1	D	213	GLY	2.3
1	H	5	THR	2.3
1	B	214	GLY	2.3
1	D	464	ALA	2.3
1	F	330	ASP	2.3
1	C	202	ASP	2.2
1	H	397	ASP	2.2
1	A	400	LYS	2.2
1	E	466	GLY	2.2
1	B	3	ASP	2.2
1	H	352	ILE	2.2
1	B	420	PRO	2.2
1	C	7	GLU	2.2
1	E	83	ASP	2.2
1	E	6	SER	2.2
1	A	5	THR	2.1
1	F	389	ARG	2.1
1	C	397	ASP	2.1
1	D	375	GLU	2.1
1	H	212	SER	2.1
1	C	402	GLY	2.1
1	C	398	ALA	2.1
1	F	344	ARG	2.1
1	E	214	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	213	GLY	2.1
1	F	203	GLY	2.1
1	C	212	SER	2.0
1	E	217	GLN	2.0
1	F	202	ASP	2.0
1	F	218	ARG	2.0
1	A	185	GLY	2.0
1	F	214	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	PG4	E	582	13/13	0.66	0.41	12.02	60,68,80,81	0
5	PG4	A	581	13/13	0.82	0.36	10.90	55,65,71,74	0
5	PG4	A	582	13/13	0.78	0.34	10.78	64,70,76,76	0
5	PG4	B	581	13/13	0.82	0.27	10.77	52,68,88,90	0
5	PG4	E	583	13/13	0.68	0.24	10.27	53,67,69,71	0
5	PG4	H	582	13/13	0.64	0.47	9.60	64,67,76,78	0
5	PG4	E	581	13/13	0.80	0.28	7.04	50,59,69,70	0
5	PG4	G	582	13/13	0.70	0.23	6.89	63,69,78,80	0
5	PG4	D	581	13/13	0.79	0.29	6.54	48,56,65,65	0
5	PG4	A	583	13/13	0.80	0.22	6.39	48,56,65,67	0
5	PG4	C	581	13/13	0.81	0.24	6.12	47,61,77,79	0
5	PG4	F	581	13/13	0.81	0.24	6.00	51,60,68,70	0
5	PG4	H	581	13/13	0.83	0.35	5.95	55,62,69,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PG4	C	582	13/13	0.79	0.27	5.26	56,66,78,79	0
6	SUC	F	591	23/23	0.79	0.21	5.21	44,64,75,82	0
5	PG4	D	582	13/13	0.80	0.33	5.10	62,68,78,81	0
5	PG4	B	582	13/13	0.79	0.24	4.99	58,61,64,65	0
5	PG4	G	581	13/13	0.75	0.24	4.66	67,69,77,78	0
6	SUC	B	591	23/23	0.71	0.21	3.66	52,66,75,77	0
6	SUC	B	592	23/23	0.82	0.27	3.61	49,56,62,67	0
4	CL	B	571	1/1	0.98	0.13	3.60	33,33,33,33	0
6	SUC	D	592	23/23	0.85	0.23	2.90	46,54,58,61	0
6	SUC	H	592	23/23	0.91	0.26	2.85	37,45,49,56	0
5	PG4	F	582	13/13	0.79	0.20	1.84	55,60,77,78	0
6	SUC	F	592	23/23	0.90	0.19	1.56	35,44,48,50	0
6	SUC	C	591	23/23	0.84	0.18	1.54	45,66,71,71	0
4	CL	D	571	1/1	0.98	0.13	1.05	33,33,33,33	0
4	CL	F	571	1/1	0.99	0.11	0.42	33,33,33,33	0
6	SUC	H	591	23/23	0.87	0.18	0.21	37,48,55,56	0
6	SUC	G	591	23/23	0.90	0.14	0.20	35,44,61,62	0
4	CL	E	571	1/1	0.99	0.12	0.17	28,28,28,28	0
4	CL	G	571	1/1	0.99	0.09	0.05	27,27,27,27	0
6	SUC	D	591	23/23	0.92	0.18	-0.22	31,43,58,65	0
2	FAD	H	551	53/53	0.97	0.11	-0.38	21,23,25,26	0
6	SUC	A	591	23/23	0.95	0.15	-0.43	33,39,46,48	0
2	FAD	F	551	53/53	0.98	0.10	-0.45	20,24,28,29	0
2	FAD	E	551	53/53	0.97	0.10	-0.49	19,24,33,34	0
2	FAD	D	551	53/53	0.97	0.10	-0.64	22,26,32,35	0
2	FAD	A	551	53/53	0.97	0.10	-0.71	20,22,24,28	0
2	FAD	B	551	53/53	0.98	0.10	-0.77	19,23,25,29	0
4	CL	C	571	1/1	0.97	0.09	-0.98	34,34,34,34	0
2	FAD	C	551	53/53	0.97	0.08	-1.19	23,26,33,38	0
2	FAD	G	551	53/53	0.98	0.09	-1.29	19,22,25,27	0
4	CL	A	571	1/1	0.99	0.09	-1.33	30,30,30,30	0
6	SUC	E	591	23/23	0.97	0.12	-1.43	26,36,44,50	0
4	CL	H	571	1/1	0.99	0.11	-1.68	34,34,34,34	0
3	NA	G	561	1/1	0.94	0.09	-3.25	26,26,26,26	0
3	NA	E	561	1/1	0.99	0.07	-4.69	23,23,23,23	0
3	NA	C	561	1/1	0.99	0.06	-5.12	22,22,22,22	0
3	NA	A	561	1/1	0.99	0.06	-6.05	23,23,23,23	0
5	PG4	B	584	13/13	0.69	0.28	-	72,85,90,91	0

6.5 Other polymers

There are no such residues in this entry.