



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2017 – 11:23 am GMT

PDB ID : 5JFM
Title : Crystal structure of Rhodopseudomonas palustris propionaldehyde dehydrogenase with bound propionyl-CoA
Authors : Zarzycki, J.; Sutter, M.; Kerfeld, C.A.
Deposited on : 2016-04-19
Resolution : 2.52 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	:	recalc29047
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)	:	recalc29047

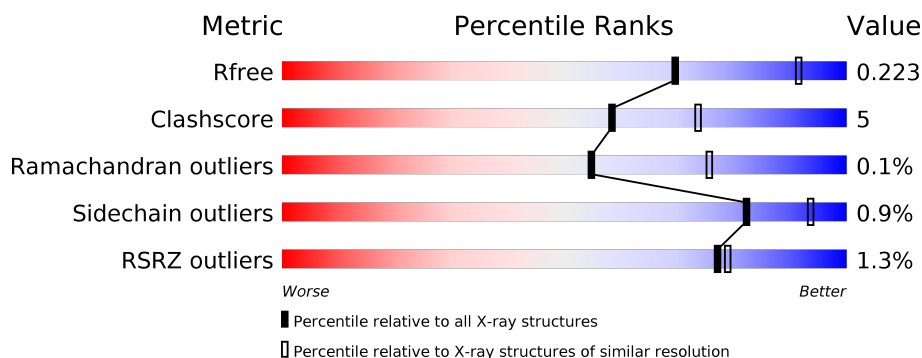
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	4636 (2.54-2.50)
Clashscore	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (2.54-2.50)
RSRZ outliers	101464	4669 (2.54-2.50)

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	524	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>16%</div> </div> </div>
1	B	524	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>14%</div> </div> </div>
1	C	524	<div> <div></div> <div> <div></div> <div>76%</div> <div>8%</div> <div>16%</div> </div> </div>
1	D	524	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>16%</div> </div> </div>
1	E	524	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>16%</div> </div> </div>
1	F	524	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	524	<p>2% 72% 12% 16%</p>
1	H	524	<p>% 71% 13% 16%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1VU	C	601	-	-	-	X
2	1VU	G	601	-	-	-	X
3	COA	B	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28030 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			
1	B	452	Total	C	N	O	S	0	1	0
			3384	2124	586	652	22			
1	C	439	Total	C	N	O	S	0	1	0
			3297	2075	570	630	22			
1	D	439	Total	C	N	O	S	0	1	0
			3297	2075	570	630	22			
1	E	439	Total	C	N	O	S	0	1	0
			3297	2075	570	630	22			
1	F	452	Total	C	N	O	S	0	0	0
			3373	2118	582	651	22			
1	G	439	Total	C	N	O	S	0	0	0
			3286	2069	566	629	22			
1	H	441	Total	C	N	O	S	0	1	0
			3307	2081	572	632	22			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q21A49
A	2	ALA	-	expression tag	UNP Q21A49
A	3	TRP	-	expression tag	UNP Q21A49
A	4	SER	-	expression tag	UNP Q21A49
A	5	HIS	-	expression tag	UNP Q21A49
A	6	PRO	-	expression tag	UNP Q21A49
A	7	GLN	-	expression tag	UNP Q21A49
A	8	PHE	-	expression tag	UNP Q21A49
A	9	GLU	-	expression tag	UNP Q21A49
A	10	LYS	-	expression tag	UNP Q21A49
A	11	GLY	-	expression tag	UNP Q21A49
A	12	HIS	-	expression tag	UNP Q21A49
A	13	MET	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASN	-	expression tag	UNP Q21A49
A	15	ASP	-	expression tag	UNP Q21A49
A	16	ALA	-	expression tag	UNP Q21A49
A	17	ASN	-	expression tag	UNP Q21A49
A	18	ILE	-	expression tag	UNP Q21A49
A	19	ALA	-	expression tag	UNP Q21A49
A	20	ASP	-	expression tag	UNP Q21A49
A	21	VAL	-	expression tag	UNP Q21A49
A	22	VAL	-	expression tag	UNP Q21A49
A	23	THR	-	expression tag	UNP Q21A49
A	24	LYS	-	expression tag	UNP Q21A49
A	25	VAL	-	expression tag	UNP Q21A49
A	26	LEU	-	expression tag	UNP Q21A49
A	27	GLY	-	expression tag	UNP Q21A49
A	28	GLU	-	expression tag	UNP Q21A49
A	29	TYR	-	expression tag	UNP Q21A49
A	30	GLY	-	expression tag	UNP Q21A49
A	31	ALA	-	expression tag	UNP Q21A49
A	32	PRO	-	expression tag	UNP Q21A49
A	33	GLY	-	expression tag	UNP Q21A49
A	34	ALA	-	expression tag	UNP Q21A49
A	35	VAL	-	expression tag	UNP Q21A49
A	36	SER	-	expression tag	UNP Q21A49
A	37	VAL	-	expression tag	UNP Q21A49
A	38	ALA	-	expression tag	UNP Q21A49
A	39	ALA	-	expression tag	UNP Q21A49
A	40	LEU	-	expression tag	UNP Q21A49
A	41	THR	-	expression tag	UNP Q21A49
A	42	ALA	-	expression tag	UNP Q21A49
A	43	LYS	-	expression tag	UNP Q21A49
A	44	SER	-	expression tag	UNP Q21A49
A	45	PRO	-	expression tag	UNP Q21A49
A	46	ASP	-	expression tag	UNP Q21A49
A	47	GLY	-	expression tag	UNP Q21A49
A	48	LYS	-	expression tag	UNP Q21A49
A	49	SER	-	expression tag	UNP Q21A49
A	50	ASN	-	expression tag	UNP Q21A49
A	51	SER	-	expression tag	UNP Q21A49
A	52	SER	-	expression tag	UNP Q21A49
A	53	ALA	-	expression tag	UNP Q21A49
A	54	ASP	-	expression tag	UNP Q21A49
A	55	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ASP	-	expression tag	UNP Q21A49
A	57	VAL	-	expression tag	UNP Q21A49
A	58	VAL	-	expression tag	UNP Q21A49
A	59	ALA	-	expression tag	UNP Q21A49
A	60	ARG	-	expression tag	UNP Q21A49
B	1	MET	-	initiating methionine	UNP Q21A49
B	2	ALA	-	expression tag	UNP Q21A49
B	3	TRP	-	expression tag	UNP Q21A49
B	4	SER	-	expression tag	UNP Q21A49
B	5	HIS	-	expression tag	UNP Q21A49
B	6	PRO	-	expression tag	UNP Q21A49
B	7	GLN	-	expression tag	UNP Q21A49
B	8	PHE	-	expression tag	UNP Q21A49
B	9	GLU	-	expression tag	UNP Q21A49
B	10	LYS	-	expression tag	UNP Q21A49
B	11	GLY	-	expression tag	UNP Q21A49
B	12	HIS	-	expression tag	UNP Q21A49
B	13	MET	-	expression tag	UNP Q21A49
B	14	ASN	-	expression tag	UNP Q21A49
B	15	ASP	-	expression tag	UNP Q21A49
B	16	ALA	-	expression tag	UNP Q21A49
B	17	ASN	-	expression tag	UNP Q21A49
B	18	ILE	-	expression tag	UNP Q21A49
B	19	ALA	-	expression tag	UNP Q21A49
B	20	ASP	-	expression tag	UNP Q21A49
B	21	VAL	-	expression tag	UNP Q21A49
B	22	VAL	-	expression tag	UNP Q21A49
B	23	THR	-	expression tag	UNP Q21A49
B	24	LYS	-	expression tag	UNP Q21A49
B	25	VAL	-	expression tag	UNP Q21A49
B	26	LEU	-	expression tag	UNP Q21A49
B	27	GLY	-	expression tag	UNP Q21A49
B	28	GLU	-	expression tag	UNP Q21A49
B	29	TYR	-	expression tag	UNP Q21A49
B	30	GLY	-	expression tag	UNP Q21A49
B	31	ALA	-	expression tag	UNP Q21A49
B	32	PRO	-	expression tag	UNP Q21A49
B	33	GLY	-	expression tag	UNP Q21A49
B	34	ALA	-	expression tag	UNP Q21A49
B	35	VAL	-	expression tag	UNP Q21A49
B	36	SER	-	expression tag	UNP Q21A49
B	37	VAL	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	ALA	-	expression tag	UNP Q21A49
B	39	ALA	-	expression tag	UNP Q21A49
B	40	LEU	-	expression tag	UNP Q21A49
B	41	THR	-	expression tag	UNP Q21A49
B	42	ALA	-	expression tag	UNP Q21A49
B	43	LYS	-	expression tag	UNP Q21A49
B	44	SER	-	expression tag	UNP Q21A49
B	45	PRO	-	expression tag	UNP Q21A49
B	46	ASP	-	expression tag	UNP Q21A49
B	47	GLY	-	expression tag	UNP Q21A49
B	48	LYS	-	expression tag	UNP Q21A49
B	49	SER	-	expression tag	UNP Q21A49
B	50	ASN	-	expression tag	UNP Q21A49
B	51	SER	-	expression tag	UNP Q21A49
B	52	SER	-	expression tag	UNP Q21A49
B	53	ALA	-	expression tag	UNP Q21A49
B	54	ASP	-	expression tag	UNP Q21A49
B	55	ALA	-	expression tag	UNP Q21A49
B	56	ASP	-	expression tag	UNP Q21A49
B	57	VAL	-	expression tag	UNP Q21A49
B	58	VAL	-	expression tag	UNP Q21A49
B	59	ALA	-	expression tag	UNP Q21A49
B	60	ARG	-	expression tag	UNP Q21A49
C	1	MET	-	initiating methionine	UNP Q21A49
C	2	ALA	-	expression tag	UNP Q21A49
C	3	TRP	-	expression tag	UNP Q21A49
C	4	SER	-	expression tag	UNP Q21A49
C	5	HIS	-	expression tag	UNP Q21A49
C	6	PRO	-	expression tag	UNP Q21A49
C	7	GLN	-	expression tag	UNP Q21A49
C	8	PHE	-	expression tag	UNP Q21A49
C	9	GLU	-	expression tag	UNP Q21A49
C	10	LYS	-	expression tag	UNP Q21A49
C	11	GLY	-	expression tag	UNP Q21A49
C	12	HIS	-	expression tag	UNP Q21A49
C	13	MET	-	expression tag	UNP Q21A49
C	14	ASN	-	expression tag	UNP Q21A49
C	15	ASP	-	expression tag	UNP Q21A49
C	16	ALA	-	expression tag	UNP Q21A49
C	17	ASN	-	expression tag	UNP Q21A49
C	18	ILE	-	expression tag	UNP Q21A49
C	19	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ASP	-	expression tag	UNP Q21A49
C	21	VAL	-	expression tag	UNP Q21A49
C	22	VAL	-	expression tag	UNP Q21A49
C	23	THR	-	expression tag	UNP Q21A49
C	24	LYS	-	expression tag	UNP Q21A49
C	25	VAL	-	expression tag	UNP Q21A49
C	26	LEU	-	expression tag	UNP Q21A49
C	27	GLY	-	expression tag	UNP Q21A49
C	28	GLU	-	expression tag	UNP Q21A49
C	29	TYR	-	expression tag	UNP Q21A49
C	30	GLY	-	expression tag	UNP Q21A49
C	31	ALA	-	expression tag	UNP Q21A49
C	32	PRO	-	expression tag	UNP Q21A49
C	33	GLY	-	expression tag	UNP Q21A49
C	34	ALA	-	expression tag	UNP Q21A49
C	35	VAL	-	expression tag	UNP Q21A49
C	36	SER	-	expression tag	UNP Q21A49
C	37	VAL	-	expression tag	UNP Q21A49
C	38	ALA	-	expression tag	UNP Q21A49
C	39	ALA	-	expression tag	UNP Q21A49
C	40	LEU	-	expression tag	UNP Q21A49
C	41	THR	-	expression tag	UNP Q21A49
C	42	ALA	-	expression tag	UNP Q21A49
C	43	LYS	-	expression tag	UNP Q21A49
C	44	SER	-	expression tag	UNP Q21A49
C	45	PRO	-	expression tag	UNP Q21A49
C	46	ASP	-	expression tag	UNP Q21A49
C	47	GLY	-	expression tag	UNP Q21A49
C	48	LYS	-	expression tag	UNP Q21A49
C	49	SER	-	expression tag	UNP Q21A49
C	50	ASN	-	expression tag	UNP Q21A49
C	51	SER	-	expression tag	UNP Q21A49
C	52	SER	-	expression tag	UNP Q21A49
C	53	ALA	-	expression tag	UNP Q21A49
C	54	ASP	-	expression tag	UNP Q21A49
C	55	ALA	-	expression tag	UNP Q21A49
C	56	ASP	-	expression tag	UNP Q21A49
C	57	VAL	-	expression tag	UNP Q21A49
C	58	VAL	-	expression tag	UNP Q21A49
C	59	ALA	-	expression tag	UNP Q21A49
C	60	ARG	-	expression tag	UNP Q21A49
D	1	MET	-	initiating methionine	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP Q21A49
D	3	TRP	-	expression tag	UNP Q21A49
D	4	SER	-	expression tag	UNP Q21A49
D	5	HIS	-	expression tag	UNP Q21A49
D	6	PRO	-	expression tag	UNP Q21A49
D	7	GLN	-	expression tag	UNP Q21A49
D	8	PHE	-	expression tag	UNP Q21A49
D	9	GLU	-	expression tag	UNP Q21A49
D	10	LYS	-	expression tag	UNP Q21A49
D	11	GLY	-	expression tag	UNP Q21A49
D	12	HIS	-	expression tag	UNP Q21A49
D	13	MET	-	expression tag	UNP Q21A49
D	14	ASN	-	expression tag	UNP Q21A49
D	15	ASP	-	expression tag	UNP Q21A49
D	16	ALA	-	expression tag	UNP Q21A49
D	17	ASN	-	expression tag	UNP Q21A49
D	18	ILE	-	expression tag	UNP Q21A49
D	19	ALA	-	expression tag	UNP Q21A49
D	20	ASP	-	expression tag	UNP Q21A49
D	21	VAL	-	expression tag	UNP Q21A49
D	22	VAL	-	expression tag	UNP Q21A49
D	23	THR	-	expression tag	UNP Q21A49
D	24	LYS	-	expression tag	UNP Q21A49
D	25	VAL	-	expression tag	UNP Q21A49
D	26	LEU	-	expression tag	UNP Q21A49
D	27	GLY	-	expression tag	UNP Q21A49
D	28	GLU	-	expression tag	UNP Q21A49
D	29	TYR	-	expression tag	UNP Q21A49
D	30	GLY	-	expression tag	UNP Q21A49
D	31	ALA	-	expression tag	UNP Q21A49
D	32	PRO	-	expression tag	UNP Q21A49
D	33	GLY	-	expression tag	UNP Q21A49
D	34	ALA	-	expression tag	UNP Q21A49
D	35	VAL	-	expression tag	UNP Q21A49
D	36	SER	-	expression tag	UNP Q21A49
D	37	VAL	-	expression tag	UNP Q21A49
D	38	ALA	-	expression tag	UNP Q21A49
D	39	ALA	-	expression tag	UNP Q21A49
D	40	LEU	-	expression tag	UNP Q21A49
D	41	THR	-	expression tag	UNP Q21A49
D	42	ALA	-	expression tag	UNP Q21A49
D	43	LYS	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	44	SER	-	expression tag	UNP Q21A49
D	45	PRO	-	expression tag	UNP Q21A49
D	46	ASP	-	expression tag	UNP Q21A49
D	47	GLY	-	expression tag	UNP Q21A49
D	48	LYS	-	expression tag	UNP Q21A49
D	49	SER	-	expression tag	UNP Q21A49
D	50	ASN	-	expression tag	UNP Q21A49
D	51	SER	-	expression tag	UNP Q21A49
D	52	SER	-	expression tag	UNP Q21A49
D	53	ALA	-	expression tag	UNP Q21A49
D	54	ASP	-	expression tag	UNP Q21A49
D	55	ALA	-	expression tag	UNP Q21A49
D	56	ASP	-	expression tag	UNP Q21A49
D	57	VAL	-	expression tag	UNP Q21A49
D	58	VAL	-	expression tag	UNP Q21A49
D	59	ALA	-	expression tag	UNP Q21A49
D	60	ARG	-	expression tag	UNP Q21A49
E	1	MET	-	initiating methionine	UNP Q21A49
E	2	ALA	-	expression tag	UNP Q21A49
E	3	TRP	-	expression tag	UNP Q21A49
E	4	SER	-	expression tag	UNP Q21A49
E	5	HIS	-	expression tag	UNP Q21A49
E	6	PRO	-	expression tag	UNP Q21A49
E	7	GLN	-	expression tag	UNP Q21A49
E	8	PHE	-	expression tag	UNP Q21A49
E	9	GLU	-	expression tag	UNP Q21A49
E	10	LYS	-	expression tag	UNP Q21A49
E	11	GLY	-	expression tag	UNP Q21A49
E	12	HIS	-	expression tag	UNP Q21A49
E	13	MET	-	expression tag	UNP Q21A49
E	14	ASN	-	expression tag	UNP Q21A49
E	15	ASP	-	expression tag	UNP Q21A49
E	16	ALA	-	expression tag	UNP Q21A49
E	17	ASN	-	expression tag	UNP Q21A49
E	18	ILE	-	expression tag	UNP Q21A49
E	19	ALA	-	expression tag	UNP Q21A49
E	20	ASP	-	expression tag	UNP Q21A49
E	21	VAL	-	expression tag	UNP Q21A49
E	22	VAL	-	expression tag	UNP Q21A49
E	23	THR	-	expression tag	UNP Q21A49
E	24	LYS	-	expression tag	UNP Q21A49
E	25	VAL	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
E	26	LEU	-	expression tag	UNP Q21A49
E	27	GLY	-	expression tag	UNP Q21A49
E	28	GLU	-	expression tag	UNP Q21A49
E	29	TYR	-	expression tag	UNP Q21A49
E	30	GLY	-	expression tag	UNP Q21A49
E	31	ALA	-	expression tag	UNP Q21A49
E	32	PRO	-	expression tag	UNP Q21A49
E	33	GLY	-	expression tag	UNP Q21A49
E	34	ALA	-	expression tag	UNP Q21A49
E	35	VAL	-	expression tag	UNP Q21A49
E	36	SER	-	expression tag	UNP Q21A49
E	37	VAL	-	expression tag	UNP Q21A49
E	38	ALA	-	expression tag	UNP Q21A49
E	39	ALA	-	expression tag	UNP Q21A49
E	40	LEU	-	expression tag	UNP Q21A49
E	41	THR	-	expression tag	UNP Q21A49
E	42	ALA	-	expression tag	UNP Q21A49
E	43	LYS	-	expression tag	UNP Q21A49
E	44	SER	-	expression tag	UNP Q21A49
E	45	PRO	-	expression tag	UNP Q21A49
E	46	ASP	-	expression tag	UNP Q21A49
E	47	GLY	-	expression tag	UNP Q21A49
E	48	LYS	-	expression tag	UNP Q21A49
E	49	SER	-	expression tag	UNP Q21A49
E	50	ASN	-	expression tag	UNP Q21A49
E	51	SER	-	expression tag	UNP Q21A49
E	52	SER	-	expression tag	UNP Q21A49
E	53	ALA	-	expression tag	UNP Q21A49
E	54	ASP	-	expression tag	UNP Q21A49
E	55	ALA	-	expression tag	UNP Q21A49
E	56	ASP	-	expression tag	UNP Q21A49
E	57	VAL	-	expression tag	UNP Q21A49
E	58	VAL	-	expression tag	UNP Q21A49
E	59	ALA	-	expression tag	UNP Q21A49
E	60	ARG	-	expression tag	UNP Q21A49
F	1	MET	-	initiating methionine	UNP Q21A49
F	2	ALA	-	expression tag	UNP Q21A49
F	3	TRP	-	expression tag	UNP Q21A49
F	4	SER	-	expression tag	UNP Q21A49
F	5	HIS	-	expression tag	UNP Q21A49
F	6	PRO	-	expression tag	UNP Q21A49
F	7	GLN	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
F	8	PHE	-	expression tag	UNP Q21A49
F	9	GLU	-	expression tag	UNP Q21A49
F	10	LYS	-	expression tag	UNP Q21A49
F	11	GLY	-	expression tag	UNP Q21A49
F	12	HIS	-	expression tag	UNP Q21A49
F	13	MET	-	expression tag	UNP Q21A49
F	14	ASN	-	expression tag	UNP Q21A49
F	15	ASP	-	expression tag	UNP Q21A49
F	16	ALA	-	expression tag	UNP Q21A49
F	17	ASN	-	expression tag	UNP Q21A49
F	18	ILE	-	expression tag	UNP Q21A49
F	19	ALA	-	expression tag	UNP Q21A49
F	20	ASP	-	expression tag	UNP Q21A49
F	21	VAL	-	expression tag	UNP Q21A49
F	22	VAL	-	expression tag	UNP Q21A49
F	23	THR	-	expression tag	UNP Q21A49
F	24	LYS	-	expression tag	UNP Q21A49
F	25	VAL	-	expression tag	UNP Q21A49
F	26	LEU	-	expression tag	UNP Q21A49
F	27	GLY	-	expression tag	UNP Q21A49
F	28	GLU	-	expression tag	UNP Q21A49
F	29	TYR	-	expression tag	UNP Q21A49
F	30	GLY	-	expression tag	UNP Q21A49
F	31	ALA	-	expression tag	UNP Q21A49
F	32	PRO	-	expression tag	UNP Q21A49
F	33	GLY	-	expression tag	UNP Q21A49
F	34	ALA	-	expression tag	UNP Q21A49
F	35	VAL	-	expression tag	UNP Q21A49
F	36	SER	-	expression tag	UNP Q21A49
F	37	VAL	-	expression tag	UNP Q21A49
F	38	ALA	-	expression tag	UNP Q21A49
F	39	ALA	-	expression tag	UNP Q21A49
F	40	LEU	-	expression tag	UNP Q21A49
F	41	THR	-	expression tag	UNP Q21A49
F	42	ALA	-	expression tag	UNP Q21A49
F	43	LYS	-	expression tag	UNP Q21A49
F	44	SER	-	expression tag	UNP Q21A49
F	45	PRO	-	expression tag	UNP Q21A49
F	46	ASP	-	expression tag	UNP Q21A49
F	47	GLY	-	expression tag	UNP Q21A49
F	48	LYS	-	expression tag	UNP Q21A49
F	49	SER	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
F	50	ASN	-	expression tag	UNP Q21A49
F	51	SER	-	expression tag	UNP Q21A49
F	52	SER	-	expression tag	UNP Q21A49
F	53	ALA	-	expression tag	UNP Q21A49
F	54	ASP	-	expression tag	UNP Q21A49
F	55	ALA	-	expression tag	UNP Q21A49
F	56	ASP	-	expression tag	UNP Q21A49
F	57	VAL	-	expression tag	UNP Q21A49
F	58	VAL	-	expression tag	UNP Q21A49
F	59	ALA	-	expression tag	UNP Q21A49
F	60	ARG	-	expression tag	UNP Q21A49
G	1	MET	-	initiating methionine	UNP Q21A49
G	2	ALA	-	expression tag	UNP Q21A49
G	3	TRP	-	expression tag	UNP Q21A49
G	4	SER	-	expression tag	UNP Q21A49
G	5	HIS	-	expression tag	UNP Q21A49
G	6	PRO	-	expression tag	UNP Q21A49
G	7	GLN	-	expression tag	UNP Q21A49
G	8	PHE	-	expression tag	UNP Q21A49
G	9	GLU	-	expression tag	UNP Q21A49
G	10	LYS	-	expression tag	UNP Q21A49
G	11	GLY	-	expression tag	UNP Q21A49
G	12	HIS	-	expression tag	UNP Q21A49
G	13	MET	-	expression tag	UNP Q21A49
G	14	ASN	-	expression tag	UNP Q21A49
G	15	ASP	-	expression tag	UNP Q21A49
G	16	ALA	-	expression tag	UNP Q21A49
G	17	ASN	-	expression tag	UNP Q21A49
G	18	ILE	-	expression tag	UNP Q21A49
G	19	ALA	-	expression tag	UNP Q21A49
G	20	ASP	-	expression tag	UNP Q21A49
G	21	VAL	-	expression tag	UNP Q21A49
G	22	VAL	-	expression tag	UNP Q21A49
G	23	THR	-	expression tag	UNP Q21A49
G	24	LYS	-	expression tag	UNP Q21A49
G	25	VAL	-	expression tag	UNP Q21A49
G	26	LEU	-	expression tag	UNP Q21A49
G	27	GLY	-	expression tag	UNP Q21A49
G	28	GLU	-	expression tag	UNP Q21A49
G	29	TYR	-	expression tag	UNP Q21A49
G	30	GLY	-	expression tag	UNP Q21A49
G	31	ALA	-	expression tag	UNP Q21A49

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Chain	Residue	Modelled	Actual	Comment	Reference
G	32	PRO	-	expression tag	UNP Q21A49
G	33	GLY	-	expression tag	UNP Q21A49
G	34	ALA	-	expression tag	UNP Q21A49
G	35	VAL	-	expression tag	UNP Q21A49
G	36	SER	-	expression tag	UNP Q21A49
G	37	VAL	-	expression tag	UNP Q21A49
G	38	ALA	-	expression tag	UNP Q21A49
G	39	ALA	-	expression tag	UNP Q21A49
G	40	LEU	-	expression tag	UNP Q21A49
G	41	THR	-	expression tag	UNP Q21A49
G	42	ALA	-	expression tag	UNP Q21A49
G	43	LYS	-	expression tag	UNP Q21A49
G	44	SER	-	expression tag	UNP Q21A49
G	45	PRO	-	expression tag	UNP Q21A49
G	46	ASP	-	expression tag	UNP Q21A49
G	47	GLY	-	expression tag	UNP Q21A49
G	48	LYS	-	expression tag	UNP Q21A49
G	49	SER	-	expression tag	UNP Q21A49
G	50	ASN	-	expression tag	UNP Q21A49
G	51	SER	-	expression tag	UNP Q21A49
G	52	SER	-	expression tag	UNP Q21A49
G	53	ALA	-	expression tag	UNP Q21A49
G	54	ASP	-	expression tag	UNP Q21A49
G	55	ALA	-	expression tag	UNP Q21A49
G	56	ASP	-	expression tag	UNP Q21A49
G	57	VAL	-	expression tag	UNP Q21A49
G	58	VAL	-	expression tag	UNP Q21A49
G	59	ALA	-	expression tag	UNP Q21A49
G	60	ARG	-	expression tag	UNP Q21A49
H	1	MET	-	initiating methionine	UNP Q21A49
H	2	ALA	-	expression tag	UNP Q21A49
H	3	TRP	-	expression tag	UNP Q21A49
H	4	SER	-	expression tag	UNP Q21A49
H	5	HIS	-	expression tag	UNP Q21A49
H	6	PRO	-	expression tag	UNP Q21A49
H	7	GLN	-	expression tag	UNP Q21A49
H	8	PHE	-	expression tag	UNP Q21A49
H	9	GLU	-	expression tag	UNP Q21A49
H	10	LYS	-	expression tag	UNP Q21A49
H	11	GLY	-	expression tag	UNP Q21A49
H	12	HIS	-	expression tag	UNP Q21A49
H	13	MET	-	expression tag	UNP Q21A49

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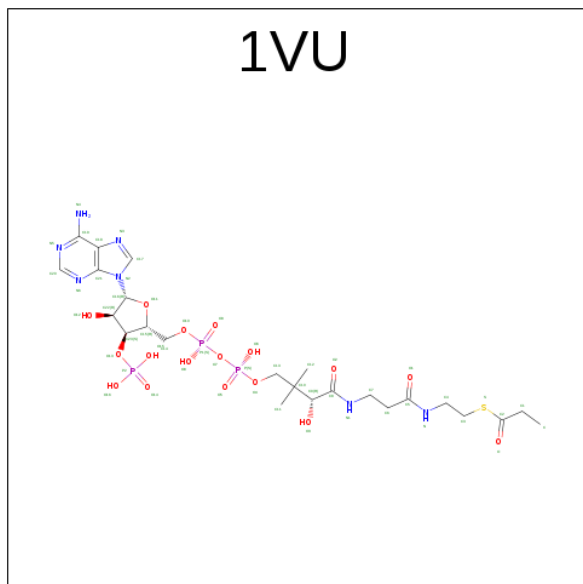
Chain	Residue	Modelled	Actual	Comment	Reference
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H	15	ASP	-	expression tag	UNP Q21A49
H	16	ALA	-	expression tag	UNP Q21A49
H	17	ASN	-	expression tag	UNP Q21A49
H	18	ILE	-	expression tag	UNP Q21A49
H	19	ALA	-	expression tag	UNP Q21A49
H	20	ASP	-	expression tag	UNP Q21A49
H	21	VAL	-	expression tag	UNP Q21A49
H	22	VAL	-	expression tag	UNP Q21A49
H	23	THR	-	expression tag	UNP Q21A49
H	24	LYS	-	expression tag	UNP Q21A49
H	25	VAL	-	expression tag	UNP Q21A49
H	26	LEU	-	expression tag	UNP Q21A49
H	27	GLY	-	expression tag	UNP Q21A49
H	28	GLU	-	expression tag	UNP Q21A49
H	29	TYR	-	expression tag	UNP Q21A49
H	30	GLY	-	expression tag	UNP Q21A49
H	31	ALA	-	expression tag	UNP Q21A49
H	32	PRO	-	expression tag	UNP Q21A49
H	33	GLY	-	expression tag	UNP Q21A49
H	34	ALA	-	expression tag	UNP Q21A49
H	35	VAL	-	expression tag	UNP Q21A49
H	36	SER	-	expression tag	UNP Q21A49
H	37	VAL	-	expression tag	UNP Q21A49
H	38	ALA	-	expression tag	UNP Q21A49
H	39	ALA	-	expression tag	UNP Q21A49
H	40	LEU	-	expression tag	UNP Q21A49
H	41	THR	-	expression tag	UNP Q21A49
H	42	ALA	-	expression tag	UNP Q21A49
H	43	LYS	-	expression tag	UNP Q21A49
H	44	SER	-	expression tag	UNP Q21A49
H	45	PRO	-	expression tag	UNP Q21A49
H	46	ASP	-	expression tag	UNP Q21A49
H	47	GLY	-	expression tag	UNP Q21A49
H	48	LYS	-	expression tag	UNP Q21A49
H	49	SER	-	expression tag	UNP Q21A49
H	50	ASN	-	expression tag	UNP Q21A49
H	51	SER	-	expression tag	UNP Q21A49
H	52	SER	-	expression tag	UNP Q21A49
H	53	ALA	-	expression tag	UNP Q21A49
H	54	ASP	-	expression tag	UNP Q21A49
H	55	ALA	-	expression tag	UNP Q21A49

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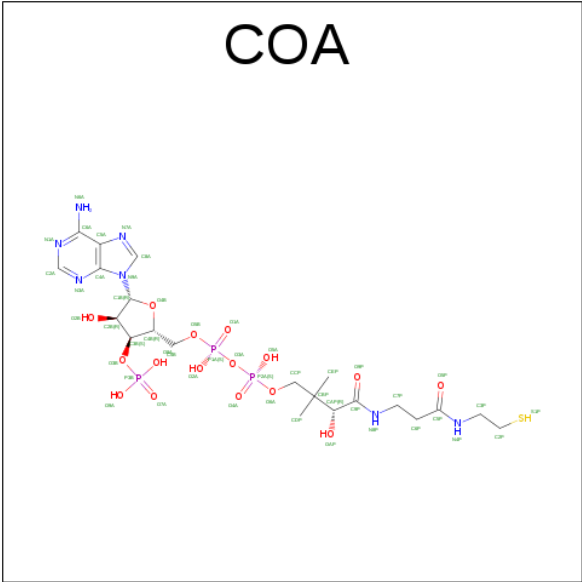
Chain	Residue	Modelled	Actual	Comment	Reference
H	56	ASP	-	expression tag	UNP Q21A49
H	57	VAL	-	expression tag	UNP Q21A49
H	58	VAL	-	expression tag	UNP Q21A49
H	59	ALA	-	expression tag	UNP Q21A49
H	60	ARG	-	expression tag	UNP Q21A49

- Molecule 2 is propionyl Coenzyme A (three-letter code: 1VU) (formula: $C_{24}H_{40}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

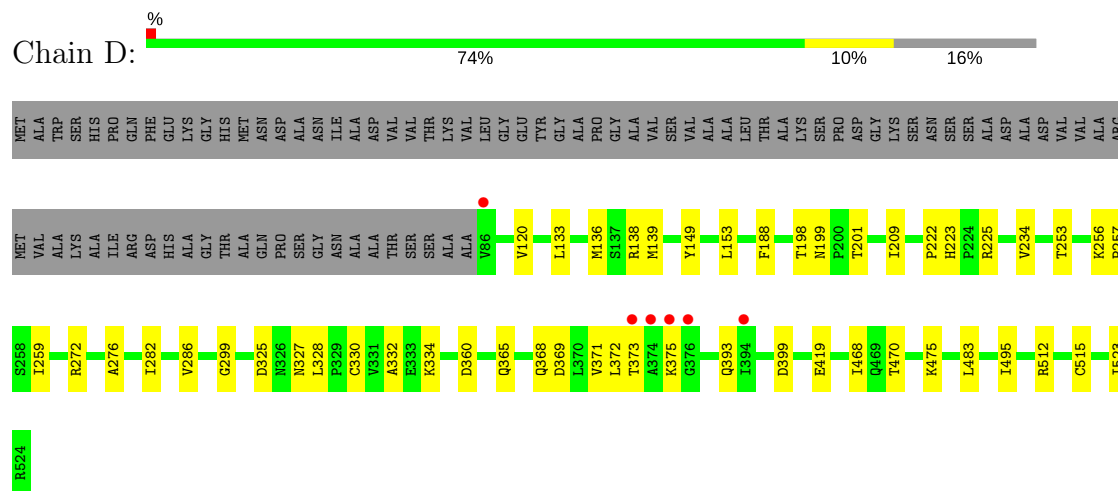


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

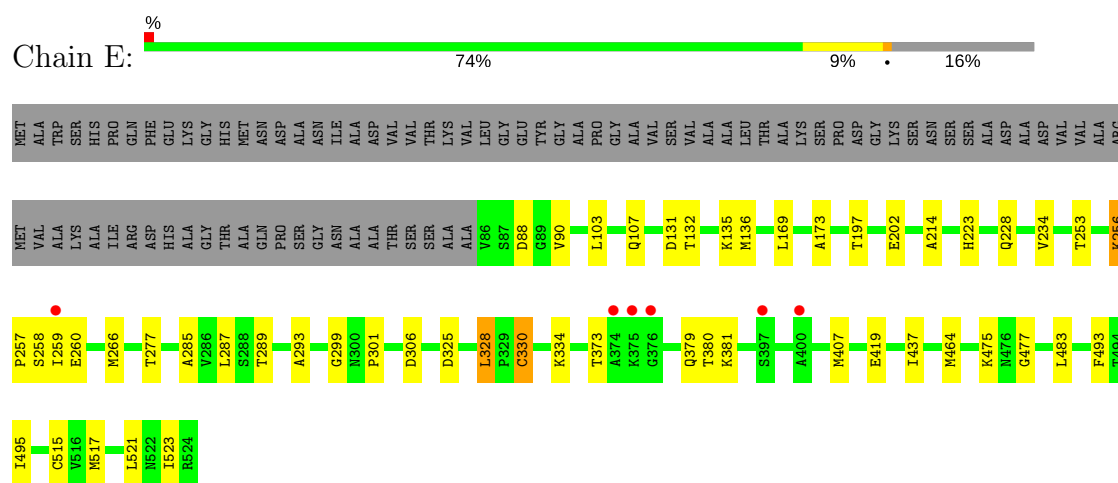
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	166	Total	O	0	0
			166	166		
4	B	160	Total	O	0	0
			160	160		
4	C	138	Total	O	0	0
			138	138		
4	D	120	Total	O	0	0
			120	120		
4	E	142	Total	O	0	0
			142	142		
4	F	141	Total	O	0	0
			141	141		
4	G	108	Total	O	0	0
			108	108		
4	H	116	Total	O	0	0
			116	116		

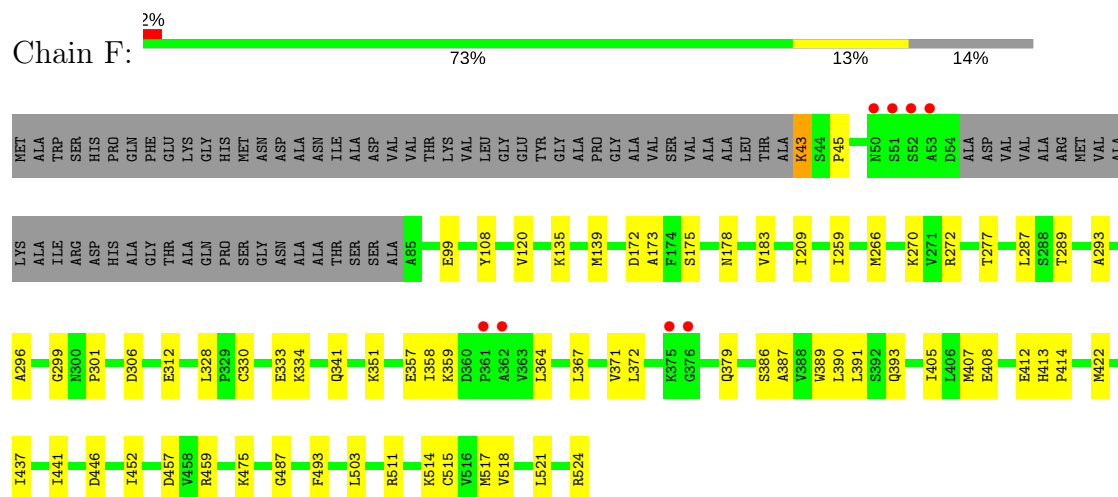
- Molecule 1: Aldehyde dehydrogenase



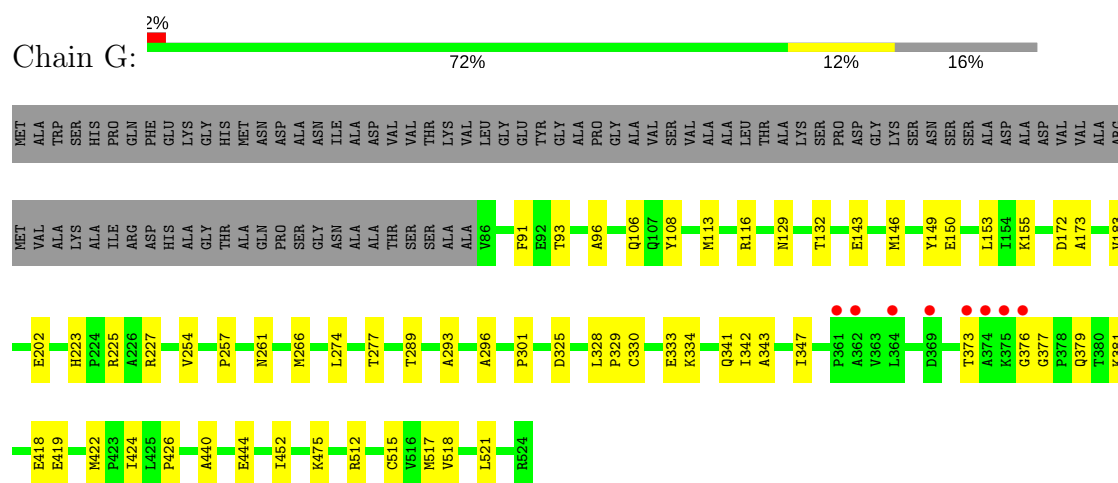
- Molecule 1: Aldehyde dehydrogenase



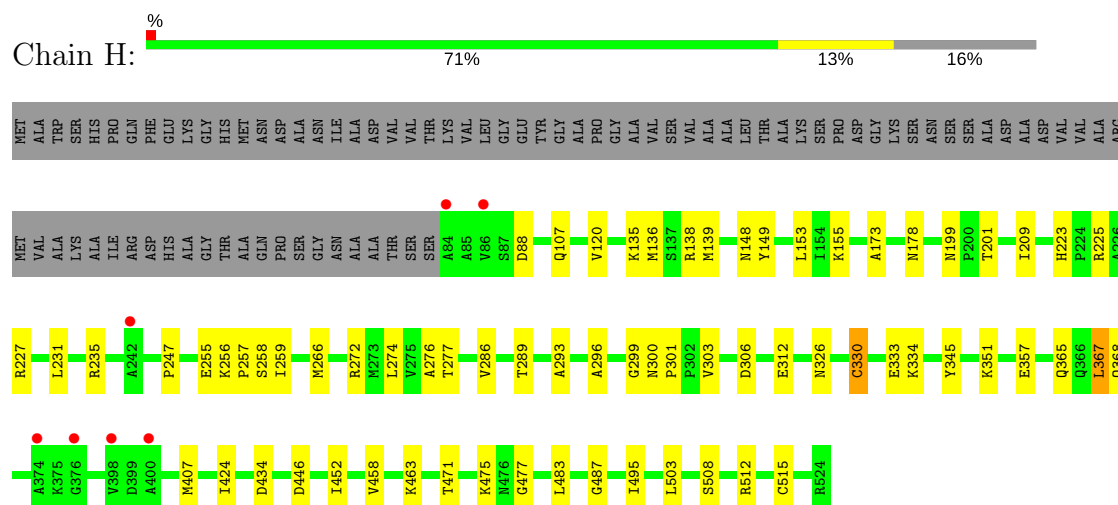
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.11Å 105.78Å 126.42Å 89.52° 71.00° 68.92°	Depositor
Resolution (Å)	39.26 – 2.52 39.26 – 2.52	Depositor EDS
% Data completeness (in resolution range)	95.5 (39.26-2.52) 85.6 (39.26-2.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.172 , 0.224 0.169 , 0.223	Depositor DCC
R_{free} test set	2002 reflections (1.48%)	DCC
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	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	0.94	EDS
Total number of atoms	28030	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, 1VU

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	0.36	1/3333 (0.0%)	0.53	1/4521 (0.0%)
1	B	0.37	1/3431 (0.0%)	0.54	1/4650 (0.0%)
1	C	0.36	0/3344	0.52	0/4535
1	D	0.34	0/3344	0.53	1/4535 (0.0%)
1	E	0.37	0/3344	0.54	1/4535 (0.0%)
1	F	0.37	0/3420	0.55	1/4636 (0.0%)
1	G	0.35	0/3333	0.53	0/4521
1	H	0.35	0/3354	0.52	1/4549 (0.0%)
All	All	0.36	2/26903 (0.0%)	0.53	6/36482 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	CYS	CB-SG	-5.09	1.73	1.81
1	B	206	CYS	CB-SG	-5.03	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	360	ASP	CB-CG-OD2	5.95	123.65	118.30
1	E	306	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	306	ASP	CB-CG-OD1	5.74	123.47	118.30
1	F	306	ASP	CB-CG-OD1	5.46	123.22	118.30
1	H	330	CYS	CA-CB-SG	5.43	123.78	114.00
1	A	306	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3286	0	3377	36	0
1	B	3384	0	3468	31	0
1	C	3297	0	3389	29	0
1	D	3297	0	3389	37	0
1	E	3297	0	3389	40	0
1	F	3373	0	3456	53	0
1	G	3286	0	3377	44	0
1	H	3307	0	3399	53	0
2	A	52	0	38	6	0
2	C	52	0	38	5	0
2	D	52	0	38	5	0
2	E	52	0	38	8	0
2	F	52	0	38	4	0
2	G	52	0	38	3	0
2	H	52	0	38	8	0
3	B	48	0	32	1	0
4	A	166	0	0	2	0
4	B	160	0	0	4	0
4	C	138	0	0	3	0
4	D	120	0	0	2	0
4	E	142	0	0	8	0
4	F	141	0	0	3	0
4	G	108	0	0	5	0
4	H	116	0	0	3	0
All	All	28030	0	27542	297	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 5.

All (297) 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:H:135:LYS:NZ	1:H:139:MET:SD	2.31	1.04
1:F:43:LYS:NZ	4:F:701:HOH:O	1.98	0.96
1:G:113:MET:SD	4:G:713:HOH:O	2.25	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:515:CYS:SG	1:H:475:LYS:NZ	2.42	0.93
1:A:475:LYS:NZ	1:C:515:CYS:SG	2.44	0.89
1:E:515:CYS:SG	1:G:475:LYS:NZ	2.47	0.88
1:F:475:LYS:NZ	1:H:515:CYS:SG	2.47	0.87
1:B:515:CYS:SG	1:D:475:LYS:NZ	2.48	0.86
1:E:334:LYS:HE2	1:E:419:GLU:HG3	1.62	0.81
1:A:515:CYS:SG	1:C:475:LYS:NZ	2.51	0.80
1:E:475:LYS:NZ	1:G:515:CYS:SG	2.55	0.78
1:C:330:CYS:H	2:C:601:1VU:H39	1.49	0.78
1:C:301:PRO:HD2	1:C:334:LYS:HD2	1.65	0.77
1:H:365:GLN:HA	1:H:368:GLN:HG3	1.68	0.76
1:H:256:LYS:HE3	1:H:258:SER:HB3	1.67	0.75
1:A:227:ARG:HD2	1:A:257:PRO:HD2	1.69	0.75
1:G:227:ARG:HG3	1:G:257:PRO:HD2	1.69	0.75
1:G:301:PRO:HD2	1:G:334:LYS:HG3	1.70	0.74
1:H:199:ASN:ND2	2:H:601:1VU:S	2.62	0.73
2:C:601:1VU:O	4:C:701:HOH:O	2.05	0.72
1:E:88:ASP:OD1	4:E:701:HOH:O	2.06	0.71
1:H:135:LYS:HG2	1:H:138:ARG:HH21	1.55	0.71
1:D:136:MET:HG3	1:D:201:THR:HG21	1.73	0.71
1:G:330:CYS:H	2:G:601:1VU:H39	1.56	0.71
1:F:446:ASP:OD2	1:H:272:ARG:NH2	2.24	0.70
1:G:129:ASN:ND2	1:G:132:THR:H	1.88	0.70
1:G:129:ASN:HD22	1:G:132:THR:H	1.37	0.70
1:F:259:ILE:HD13	2:F:601:1VU:H6	1.74	0.69
1:H:303:VAL:HG22	1:H:452:ILE:HB	1.75	0.69
1:A:523:ILE:O	1:B:513:ARG:NH2	2.26	0.69
1:B:475:LYS:NZ	1:D:515:CYS:SG	2.58	0.68
1:D:259:ILE:HD12	2:D:601:1VU:H6	1.75	0.68
1:A:266:MET:HB3	1:A:289:THR:HG21	1.76	0.67
1:E:330:CYS:H	2:E:601:1VU:H36	1.59	0.67
1:F:277:THR:HA	1:F:296:ALA:HB3	1.78	0.66
1:F:330:CYS:H	2:F:601:1VU:H40	1.58	0.66
1:F:328:LEU:O	4:F:702:HOH:O	2.12	0.65
1:F:301:PRO:HD2	1:F:334:LYS:HD2	1.78	0.65
1:A:278:GLY:HA2	2:A:601:1VU:H30	1.80	0.64
1:H:299:GLY:O	1:H:301:PRO:HD3	1.98	0.64
1:D:199:ASN:ND2	2:D:601:1VU:S	2.70	0.64
1:F:364:LEU:HD21	1:F:413:HIS:HE2	1.63	0.64
1:E:258:SER:OG	1:E:260:GLU:HG3	1.97	0.63
1:E:301:PRO:HD2	1:E:334:LYS:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:523:ILE:HG13	4:E:753:HOH:O	1.97	0.63
1:G:333:GLU:HG3	1:G:452:ILE:HD13	1.81	0.63
1:H:107:GLN:NE2	4:H:701:HOH:O	2.31	0.63
1:E:517:MET:HE3	1:H:458:VAL:HG21	1.80	0.63
1:F:386:SER:O	1:F:390:LEU:HD12	1.98	0.62
1:F:359:LYS:NZ	1:F:408:GLU:H	1.97	0.62
1:H:227:ARG:HB2	1:H:257:PRO:HG2	1.80	0.62
1:G:146:MET:HB3	1:G:328:LEU:HD11	1.82	0.62
1:B:483:LEU:HD21	1:B:495:ILE:HD11	1.81	0.62
1:D:393:GLN:NE2	4:D:703:HOH:O	2.31	0.62
1:H:368:GLN:NE2	4:H:702:HOH:O	2.33	0.62
1:C:259:ILE:HD13	2:C:601:1VU:H6	1.83	0.61
1:C:118:ARG:NH2	1:C:244:LEU:O	2.33	0.61
1:F:120:VAL:HG13	1:F:209:ILE:HG23	1.82	0.61
1:A:195:THR:O	2:A:601:1VU:N4	2.34	0.60
1:H:223:HIS:NE2	2:H:601:1VU:O5	2.23	0.60
1:B:301:PRO:HD2	1:B:334:LYS:HD2	1.83	0.60
1:H:136:MET:HG3	1:H:201:THR:HG21	1.83	0.60
1:H:231:LEU:HD21	1:H:255:GLU:HA	1.84	0.60
1:E:259:ILE:HD12	2:E:601:1VU:H6	1.83	0.60
1:C:277:THR:HG22	2:C:601:1VU:H32	1.85	0.59
1:B:328:LEU:HD11	1:B:384:GLY:HA3	1.83	0.59
1:F:351:LYS:HD2	1:F:357:GLU:OE1	2.01	0.59
1:F:299:GLY:O	1:F:301:PRO:HD3	2.03	0.58
1:F:359:LYS:HZ3	1:F:408:GLU:H	1.52	0.58
1:A:228:GLN:HG3	1:F:341:GLN:HB3	1.86	0.58
1:C:513:ARG:NH1	1:D:523:ILE:O	2.37	0.57
1:D:198:THR:HB	1:D:328:LEU:HG	1.86	0.57
1:A:227:ARG:NH1	1:A:255:GLU:O	2.37	0.56
1:G:261:ASN:ND2	4:G:705:HOH:O	2.37	0.56
1:H:301:PRO:HD2	1:H:334:LYS:HG3	1.87	0.56
2:E:601:1VU:O3	2:E:601:1VU:O9	2.24	0.56
1:H:225:ARG:NH2	2:H:601:1VU:O9	2.39	0.56
1:E:234:VAL:HG11	1:E:253:THR:HG22	1.86	0.56
1:F:367:LEU:O	1:F:371:VAL:HG22	2.05	0.56
1:F:175:SER:O	1:F:524:ARG:NH2	2.38	0.56
1:E:90:VAL:O	4:E:701:HOH:O	2.18	0.55
1:E:330:CYS:SG	2:E:601:1VU:H35	2.46	0.55
1:B:333:GLU:OE2	1:B:333:GLU:N	2.34	0.55
1:A:260:GLU:N	1:A:260:GLU:OE1	2.38	0.55
1:H:330:CYS:H	2:H:601:1VU:H40	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:GLU:N	1:G:333:GLU:OE1	2.31	0.55
1:G:379:GLN:HG3	1:G:381:LYS:HG3	1.88	0.54
1:B:414:PRO:O	1:B:418:GLU:HG2	2.08	0.54
1:G:173:ALA:HB2	1:H:173:ALA:HB2	1.87	0.54
1:G:334:LYS:HE3	1:G:419:GLU:HG3	1.90	0.54
1:E:169:LEU:HD11	1:E:214:ALA:HA	1.90	0.54
1:H:434:ASP:OD1	1:H:463:LYS:NZ	2.37	0.54
1:B:266:MET:HB3	1:B:289:THR:HG21	1.89	0.54
1:C:330:CYS:SG	2:C:601:1VU:H33	2.48	0.53
1:D:365:GLN:NE2	1:D:365:GLN:O	2.39	0.53
1:E:380:THR:HB	4:E:827:HOH:O	2.09	0.53
1:H:155:LYS:NZ	1:H:199:ASN:OD1	2.20	0.53
1:H:120:VAL:HG13	1:H:209:ILE:HG23	1.91	0.53
1:G:149:TYR:CZ	1:G:153:LEU:HD11	2.44	0.53
1:G:143:GLU:HG2	1:G:225:ARG:O	2.09	0.53
1:E:483:LEU:HD21	1:E:495:ILE:HD11	1.90	0.53
1:G:325:ASP:HB3	1:G:329:PRO:HD3	1.91	0.53
1:C:461:LEU:HD22	1:C:475:LYS:HG2	1.90	0.53
1:F:99:GLU:OE1	1:F:270:LYS:NZ	2.39	0.53
1:G:517:MET:HG2	1:G:521:LEU:HD12	1.91	0.53
1:H:330:CYS:SG	2:H:601:1VU:H32	2.49	0.53
1:C:333:GLU:HG3	1:C:452:ILE:HD13	1.90	0.52
1:E:228:GLN:NE2	4:E:704:HOH:O	2.36	0.52
1:G:223:HIS:CE1	1:G:225:ARG:HE	2.27	0.52
1:D:375:LYS:H	1:D:375:LYS:HD2	1.75	0.52
1:A:517:MET:HG2	1:A:521:LEU:HD12	1.92	0.52
1:B:172:ASP:HB2	1:B:183:VAL:HB	1.92	0.52
1:G:277:THR:HG22	2:G:601:1VU:H34	1.91	0.52
1:H:259:ILE:HD11	2:H:601:1VU:H6	1.90	0.52
2:E:601:1VU:H34	4:E:703:HOH:O	2.09	0.51
1:G:155:LYS:NZ	1:G:202:GLU:OE2	2.43	0.51
1:C:325:ASP:O	1:C:328:LEU:HB2	2.11	0.51
1:D:483:LEU:HD11	2:D:601:1VU:H38	1.92	0.51
1:G:422:MET:HE2	1:G:424:ILE:HD12	1.92	0.51
1:H:148:ASN:ND2	1:H:326:ASN:OD1	2.40	0.51
1:H:277:THR:HA	1:H:296:ALA:HB2	1.92	0.51
1:D:138:ARG:HB3	1:D:149:TYR:CD1	2.46	0.51
1:C:120:VAL:HG13	1:C:209:ILE:HG23	1.92	0.51
1:H:351:LYS:HD3	1:H:357:GLU:HB2	1.91	0.51
1:H:503:LEU:HD12	4:H:732:HOH:O	2.10	0.51
1:A:330:CYS:HB2	2:A:601:1VU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:MET:HG2	1:B:521:LEU:HD12	1.92	0.51
1:G:150:GLU:HA	1:G:153:LEU:HD12	1.93	0.50
1:D:234:VAL:HG11	1:D:253:THR:HG22	1.94	0.50
1:D:332:ALA:O	1:D:334:LYS:HG3	2.11	0.50
1:H:266:MET:HB3	1:H:289:THR:HG21	1.94	0.50
1:A:330:CYS:SG	2:A:601:1VU:H32	2.51	0.50
1:C:341:GLN:OE1	1:C:341:GLN:N	2.45	0.50
1:B:198:THR:HG21	4:B:703:HOH:O	2.12	0.49
1:E:325:ASP:O	1:E:328:LEU:HB2	2.11	0.49
1:B:333:GLU:HG3	1:B:452:ILE:HD13	1.94	0.49
1:D:330:CYS:HB2	2:D:601:1VU:O	2.11	0.49
1:A:227:ARG:HB2	1:A:257:PRO:HG2	1.94	0.49
1:A:262:THR:OG1	2:A:601:1VU:H7	2.12	0.49
1:F:517:MET:HG2	1:F:521:LEU:HD12	1.93	0.49
1:E:517:MET:HG2	1:E:521:LEU:HD12	1.94	0.49
1:A:138:ARG:NH2	1:F:312:GLU:OE2	2.45	0.49
1:F:266:MET:HB3	1:F:289:THR:HG21	1.95	0.49
1:A:287:LEU:HD23	1:A:293:ALA:HB3	1.95	0.49
1:D:375:LYS:H	1:D:375:LYS:CD	2.26	0.49
1:F:514:LYS:HD2	1:H:503:LEU:CD1	2.43	0.49
1:C:172:ASP:HB2	1:C:183:VAL:HB	1.94	0.48
1:C:318:ILE:HG21	1:C:336:ILE:HD11	1.94	0.48
1:A:197:THR:HB	1:A:223:HIS:CG	2.48	0.48
1:H:367:LEU:HD21	1:H:424:ILE:HD13	1.94	0.48
1:E:330:CYS:H	2:E:601:1VU:C1	2.26	0.48
1:G:93:THR:HG23	1:G:96:ALA:HB3	1.95	0.48
1:A:499:THR:HA	1:C:292:LYS:HD2	1.94	0.48
1:F:371:VAL:C	1:F:379:GLN:HG3	2.34	0.48
1:A:259:ILE:HG22	2:A:601:1VU:N6	2.29	0.48
1:H:149:TYR:CZ	1:H:153:LEU:HD11	2.48	0.48
1:A:409:VAL:O	4:A:702:HOH:O	2.20	0.48
1:D:334:LYS:HD2	1:D:419:GLU:OE2	2.13	0.48
1:D:223:HIS:ND1	1:D:225:ARG:HG2	2.29	0.48
1:F:493:PHE:HD1	2:F:601:1VU:H37	1.79	0.48
1:H:303:VAL:HG21	1:H:333:GLU:CG	2.43	0.47
1:F:178:ASN:HB3	1:H:487:GLY:HA2	1.96	0.47
1:H:88:ASP:OD2	1:H:235:ARG:NH1	2.48	0.47
1:B:263:ASN:HA	1:B:266:MET:HE2	1.96	0.47
1:B:446:ASP:OD2	1:D:272:ARG:NH2	2.46	0.47
1:F:301:PRO:CD	1:F:334:LYS:HD2	2.43	0.47
1:A:415:PHE:CD1	1:A:420:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:ILE:O	1:F:359:LYS:HE2	2.15	0.47
1:B:368:GLN:OE1	1:B:413:HIS:NE2	2.44	0.47
1:D:373:THR:OG1	1:D:375:LYS:HD3	2.15	0.47
1:F:389:TRP:O	1:F:393:GLN:HG2	2.15	0.47
1:A:116:ARG:NH2	4:A:716:HOH:O	2.45	0.47
1:F:413:HIS:CG	1:F:414:PRO:HD2	2.49	0.47
1:A:523:ILE:HG13	4:B:702:HOH:O	2.15	0.47
2:D:601:1VU:O6	2:D:601:1VU:H10	2.15	0.47
1:E:266:MET:HB3	1:E:289:THR:HG21	1.96	0.47
1:B:523:ILE:HG13	4:B:734:HOH:O	2.14	0.47
1:A:347:ILE:HG22	1:A:351:LYS:HE2	1.97	0.46
1:E:287:LEU:HD23	1:E:293:ALA:HB3	1.97	0.46
1:G:172:ASP:HB2	1:G:183:VAL:HB	1.97	0.46
1:C:115:ASP:OD1	1:C:118:ARG:NH1	2.47	0.46
1:E:477:GLY:HA3	1:G:518:VAL:HG21	1.96	0.46
1:D:483:LEU:HD21	1:D:495:ILE:HD11	1.98	0.46
1:H:303:VAL:HG21	1:H:333:GLU:HG3	1.98	0.46
1:D:327:ASN:OD1	1:D:334:LYS:HE3	2.15	0.46
1:D:468:ILE:HG23	1:D:470:THR:HG23	1.98	0.46
1:F:272:ARG:NH2	1:H:446:ASP:OD2	2.49	0.46
1:G:113:MET:HA	4:G:713:HOH:O	2.15	0.46
1:H:107:GLN:HG3	1:H:247:PRO:HB3	1.97	0.46
1:E:135:LYS:NZ	4:E:716:HOH:O	2.49	0.46
1:F:172:ASP:HB2	1:F:183:VAL:HB	1.97	0.46
1:F:371:VAL:HG23	1:F:372:LEU:CD1	2.46	0.45
1:F:45:PRO:HA	1:G:341:GLN:HG3	1.97	0.45
1:F:487:GLY:HA2	1:H:178:ASN:HB3	1.98	0.45
1:F:287:LEU:HD23	1:F:293:ALA:HB3	1.97	0.45
1:G:440:ALA:O	1:G:444:GLU:HB2	2.16	0.45
1:A:328:LEU:N	1:A:329:PRO:HD2	2.31	0.45
1:D:120:VAL:HG13	1:D:209:ILE:HG23	1.99	0.45
1:F:457:ASP:OD1	1:F:459:ARG:HD3	2.15	0.45
1:H:259:ILE:HG12	2:H:601:1VU:N6	2.32	0.45
1:H:312:GLU:OE2	1:H:345:TYR:OH	2.20	0.45
1:H:483:LEU:HD21	1:H:495:ILE:HD11	1.97	0.45
1:C:512[A]:ARG:NH2	4:C:711:HOH:O	2.45	0.45
1:E:103:LEU:O	1:E:107:GLN:HG3	2.16	0.45
1:F:514:LYS:HD2	1:H:503:LEU:HD13	1.99	0.45
1:D:138:ARG:HB3	1:D:149:TYR:HD1	1.82	0.45
1:A:301:PRO:HD2	1:A:334:LYS:HD2	1.98	0.45
1:D:299:GLY:N	4:D:718:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:VAL:HG13	1:C:295:GLY:HA3	1.99	0.44
1:C:282:ILE:HA	1:C:282:ILE:HD12	1.82	0.44
1:E:173:ALA:HB2	1:F:173:ALA:HB2	1.99	0.44
1:D:368:GLN:HB3	1:D:372:LEU:HD12	2.00	0.44
1:C:205:VAL:O	1:C:209:ILE:HG13	2.18	0.44
1:D:328:LEU:HA	1:D:328:LEU:HD12	1.88	0.44
1:G:373:THR:HG22	1:G:377:GLY:O	2.18	0.44
1:E:301:PRO:HD2	1:E:334:LYS:CG	2.44	0.44
1:H:276:ALA:HB2	1:H:286:VAL:HG11	1.99	0.44
1:B:172:ASP:OD2	1:B:512[B]:ARG:NH1	2.51	0.44
1:F:357:GLU:OE2	1:F:359:LYS:HE3	2.18	0.44
1:C:105:GLN:HG3	1:C:189:GLY:O	2.17	0.43
1:G:334:LYS:CE	1:G:419:GLU:HG3	2.48	0.43
1:E:256:LYS:HA	1:E:256:LYS:HD2	1.41	0.43
1:E:437:ILE:HG12	1:E:464:MET:HB2	2.00	0.43
1:F:503:LEU:O	1:H:512[A]:ARG:NH2	2.51	0.43
1:C:367:LEU:O	1:C:371:VAL:HG22	2.18	0.43
1:B:134:GLU:HG2	1:B:149:TYR:OH	2.19	0.43
1:E:285:ALA:O	1:E:289:THR:HG23	2.18	0.43
1:C:169:LEU:HD11	1:C:214:ALA:HA	2.00	0.43
1:D:371:VAL:HG23	1:D:372:LEU:HG	2.00	0.43
1:F:437:ILE:O	1:F:441:ILE:HG13	2.17	0.43
1:D:325:ASP:O	1:D:328:LEU:HB2	2.19	0.43
1:G:277:THR:HA	1:G:296:ALA:HB3	2.00	0.43
1:A:187:PRO:HG3	1:A:215:GLY:HA3	2.00	0.43
1:E:197:THR:HB	1:E:223:HIS:CG	2.54	0.43
1:F:371:VAL:HB	1:F:422:MET:SD	2.59	0.43
1:H:227:ARG:CB	1:H:257:PRO:HG2	2.48	0.43
1:B:168:ASP:HB3	1:B:506:ALA:HB3	2.01	0.43
1:C:429:ARG:NH1	4:C:705:HOH:O	2.41	0.43
1:F:371:VAL:HG23	1:F:372:LEU:HD12	2.00	0.43
1:B:365:GLN:NE2	1:B:369:ASP:OD1	2.52	0.43
1:E:373:THR:HG22	1:E:379:GLN:OE1	2.19	0.42
1:F:387:ALA:HB1	1:F:405:ILE:CD1	2.50	0.42
1:F:511:ARG:NH2	1:H:471:THR:OG1	2.52	0.42
1:B:277:THR:HA	1:B:296:ALA:HB3	2.02	0.42
1:B:422:MET:O	1:B:424:ILE:N	2.47	0.42
1:D:222:PRO:HG2	1:D:257:PRO:HG3	2.01	0.42
1:E:407:MET:N	1:E:407:MET:SD	2.93	0.42
1:E:202:GLU:HB3	1:E:493:PHE:CD2	2.54	0.42
1:A:381:LYS:HE2	1:A:381:LYS:HB2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:LEU:HG	1:F:405:ILE:HD11	2.00	0.42
1:G:106:GLN:NE2	4:G:712:HOH:O	2.52	0.42
1:G:343:ALA:O	1:G:347:ILE:HG13	2.19	0.42
1:G:376:GLY:O	1:G:418:GLU:HG3	2.20	0.42
1:G:334:LYS:O	1:G:426:PRO:HD2	2.20	0.42
1:G:266:MET:HB3	1:G:289:THR:HG21	2.00	0.42
1:A:372:LEU:HD22	1:A:376:GLY:O	2.20	0.42
1:D:133:LEU:HG	1:D:153:LEU:CD2	2.50	0.42
1:E:381:LYS:HE2	1:E:381:LYS:HB2	1.67	0.42
2:E:601:1VU:P1	2:E:601:1VU:H25	2.41	0.42
1:F:412:GLU:OE2	4:F:703:HOH:O	2.21	0.42
1:B:511:ARG:HD3	4:B:745:HOH:O	2.19	0.41
1:A:475:LYS:HE3	1:C:517:MET:HB2	2.03	0.41
1:F:330:CYS:HG	2:F:601:1VU:C2	2.33	0.41
1:F:333:GLU:HG3	1:F:452:ILE:HD13	2.02	0.41
1:A:373:THR:OG1	1:A:375:LYS:HB2	2.20	0.41
1:B:444:GLU:OE1	1:B:448:ARG:N	2.48	0.41
1:E:334:LYS:HB3	4:E:737:HOH:O	2.20	0.41
1:H:155:LYS:HE2	1:H:155:LYS:HB3	1.90	0.41
1:B:278:GLY:HA2	3:B:601:COA:H62	2.02	0.41
1:D:276:ALA:HB2	1:D:286:VAL:HG11	2.02	0.41
1:A:173:ALA:HB2	1:B:173:ALA:HB2	2.02	0.41
1:G:342:ILE:H	1:G:342:ILE:HG13	1.79	0.41
1:D:282:ILE:HA	1:D:282:ILE:HD12	1.84	0.41
1:G:116:ARG:NE	4:G:713:HOH:O	2.54	0.41
1:A:364:LEU:O	1:A:368:GLN:HG3	2.21	0.41
1:B:328:LEU:HD11	1:B:384:GLY:CA	2.49	0.41
1:F:518:VAL:HG21	1:H:477:GLY:HA3	2.03	0.41
1:B:103:LEU:O	1:B:107:GLN:HG3	2.21	0.41
1:E:277:THR:HG22	2:E:601:1VU:H32	2.02	0.41
1:E:299:GLY:C	1:E:301:PRO:HD3	2.41	0.41
1:G:330:CYS:SG	2:G:601:1VU:H32	2.60	0.41
1:C:287:LEU:HD23	1:C:293:ALA:HB3	2.03	0.41
1:D:365:GLN:NE2	1:D:369:ASP:OD1	2.53	0.41
1:B:204:ILE:O	1:B:208:SER:OG	2.33	0.41
1:E:328:LEU:HD12	1:E:328:LEU:HA	1.92	0.41
1:G:274:LEU:O	1:G:293:ALA:HA	2.21	0.41
1:G:225:ARG:H	1:G:225:ARG:HG3	1.57	0.40
1:A:459:ARG:HE	1:A:459:ARG:HB2	1.71	0.40
1:B:120:VAL:HG13	1:B:209:ILE:HG23	2.02	0.40
1:D:225:ARG:HG2	1:D:225:ARG:H	1.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ASP:N	1:D:399:ASP:OD1	2.46	0.40
1:E:132:THR:O	1:E:136:MET:HG2	2.21	0.40
1:A:292:LYS:HD3	1:C:499:THR:HA	2.02	0.40
1:F:135:LYS:O	1:F:139:MET:HB2	2.21	0.40
1:G:91:PHE:O	1:G:254:VAL:HA	2.22	0.40
1:H:274:LEU:O	1:H:293:ALA:HA	2.21	0.40
1:H:330:CYS:N	2:H:601:1VU:H40	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/524 (83%)	433 (99%)	4 (1%)	0	100	100
1	B	449/524 (86%)	442 (98%)	7 (2%)	0	100	100
1	C	438/524 (84%)	433 (99%)	5 (1%)	0	100	100
1	D	438/524 (84%)	434 (99%)	4 (1%)	0	100	100
1	E	438/524 (84%)	432 (99%)	5 (1%)	1 (0%)	51	72
1	F	448/524 (86%)	440 (98%)	8 (2%)	0	100	100
1	G	437/524 (83%)	427 (98%)	10 (2%)	0	100	100
1	H	440/524 (84%)	431 (98%)	8 (2%)	1 (0%)	51	72
All	All	3525/4192 (84%)	3472 (98%)	51 (1%)	2 (0%)	55	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	257	PRO
1	H	300	ASN

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	358/417 (86%)	356 (99%)	2 (1%)	89	96
1	B	369/417 (88%)	366 (99%)	3 (1%)	85	94
1	C	359/417 (86%)	355 (99%)	4 (1%)	78	91
1	D	359/417 (86%)	354 (99%)	5 (1%)	71	89
1	E	359/417 (86%)	355 (99%)	4 (1%)	78	91
1	F	368/417 (88%)	365 (99%)	3 (1%)	85	94
1	G	358/417 (86%)	356 (99%)	2 (1%)	89	96
1	H	359/417 (86%)	355 (99%)	4 (1%)	78	91
All	All	2889/3336 (87%)	2862 (99%)	27 (1%)	82	93

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	LYS
1	A	407	MET
1	B	108	TYR
1	B	240	LYS
1	B	330	CYS
1	C	118	ARG
1	C	188	PHE
1	C	328	LEU
1	C	407	MET
1	D	139	MET
1	D	188	PHE
1	D	256	LYS
1	D	512[A]	ARG
1	D	512[B]	ARG
1	E	131	ASP
1	E	256	LYS
1	E	328	LEU
1	E	330	CYS
1	F	43	LYS

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Mol	Chain	Res	Type
1	F	108	TYR
1	F	407	MET
1	G	108	TYR
1	G	512	ARG
1	H	306	ASP
1	H	367	LEU
1	H	407	MET
1	H	508	SER

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	365	GLN
1	C	105	GLN
1	F	50	ASN
1	G	129	ASN
1	H	366	GLN
1	H	368	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1VU	A	601	-	47,54,54	3.36	11 (23%)	54,80,80	2.07	10 (18%)
3	COA	B	601	-	43,50,50	3.48	12 (27%)	48,75,75	1.78	4 (8%)
2	1VU	C	601	-	47,54,54	3.35	12 (25%)	54,80,80	2.32	8 (14%)
2	1VU	D	601	-	47,54,54	3.39	13 (27%)	54,80,80	1.93	8 (14%)
2	1VU	E	601	-	47,54,54	3.28	12 (25%)	54,80,80	2.23	13 (24%)
2	1VU	F	601	-	47,54,54	3.35	12 (25%)	54,80,80	2.41	8 (14%)
2	1VU	G	601	-	47,54,54	3.29	12 (25%)	54,80,80	2.36	14 (25%)
2	1VU	H	601	-	47,54,54	3.46	15 (31%)	54,80,80	2.52	11 (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	1VU	A	601	-	-	0/48/69/69	0/3/3/3
3	COA	B	601	-	-	0/44/64/64	0/3/3/3
2	1VU	C	601	-	-	0/48/69/69	0/3/3/3
2	1VU	D	601	-	-	1/48/69/69	0/3/3/3
2	1VU	E	601	-	-	0/48/69/69	0/3/3/3
2	1VU	F	601	-	-	2/48/69/69	0/3/3/3
2	1VU	G	601	-	-	2/48/69/69	0/3/3/3
2	1VU	H	601	-	-	0/48/69/69	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	1VU	C22-C16	-12.27	1.34	1.53
2	C	601	1VU	C22-C16	-12.24	1.34	1.53
2	D	601	1VU	C22-C16	-12.05	1.34	1.53
3	B	601	COA	C2B-C1B	-11.97	1.34	1.53
2	A	601	1VU	C22-C16	-11.91	1.34	1.53
2	F	601	1VU	C22-C16	-11.76	1.35	1.53
2	G	601	1VU	C22-C16	-11.44	1.35	1.53
2	E	601	1VU	C22-C16	-11.41	1.35	1.53
2	C	601	1VU	O11-C15	-6.04	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	1VU	O11-C15	-6.03	1.31	1.45
2	H	601	1VU	O11-C15	-5.96	1.31	1.45
2	D	601	1VU	O11-C15	-5.91	1.31	1.45
2	E	601	1VU	O11-C15	-5.80	1.31	1.45
3	B	601	COA	O4B-C4B	-5.72	1.32	1.45
2	G	601	1VU	O11-C15	-5.72	1.32	1.45
2	A	601	1VU	O11-C15	-5.64	1.32	1.45
2	H	601	1VU	C1-C2	-4.21	1.44	1.51
2	H	601	1VU	O-C2	-2.77	1.16	1.21
2	D	601	1VU	O3-C9	-2.58	1.37	1.42
2	E	601	1VU	O3-C9	-2.54	1.37	1.42
3	B	601	COA	OAP-CAP	-2.48	1.37	1.42
2	H	601	1VU	C2-S	-2.45	1.71	1.76
2	A	601	1VU	O3-C9	-2.42	1.37	1.42
2	F	601	1VU	O3-C9	-2.39	1.37	1.42
2	H	601	1VU	O3-C9	-2.31	1.37	1.42
2	C	601	1VU	C18-C21	-2.30	1.35	1.40
2	G	601	1VU	O3-C9	-2.29	1.37	1.42
2	C	601	1VU	O3-C9	-2.29	1.37	1.42
2	D	601	1VU	C18-C21	-2.23	1.35	1.40
2	D	601	1VU	O13-C23	-2.21	1.35	1.44
2	F	601	1VU	C18-C21	-2.20	1.35	1.40
3	B	601	COA	C5A-C4A	-2.19	1.35	1.40
3	B	601	COA	O3B-C3B	-2.13	1.36	1.44
2	F	601	1VU	O13-C23	-2.10	1.36	1.44
2	H	601	1VU	O13-C23	-2.09	1.36	1.44
2	A	601	1VU	C18-C21	-2.08	1.35	1.40
2	C	601	1VU	O13-C23	-2.05	1.36	1.44
2	G	601	1VU	C18-C21	-2.05	1.35	1.40
2	E	601	1VU	C18-C21	-2.03	1.35	1.40
2	H	601	1VU	C18-C21	-2.01	1.36	1.40
2	G	601	1VU	O12-C22	2.01	1.47	1.43
2	A	601	1VU	O-C2	2.04	1.24	1.21
2	F	601	1VU	O12-C22	2.05	1.47	1.43
2	H	601	1VU	O12-C22	2.07	1.47	1.43
2	D	601	1VU	O-C2	2.08	1.24	1.21
3	B	601	COA	O2B-C2B	2.08	1.47	1.43
2	E	601	1VU	O-C2	2.11	1.24	1.21
2	D	601	1VU	O12-C22	2.11	1.47	1.43
2	E	601	1VU	O12-C22	2.16	1.47	1.43
2	C	601	1VU	C20-N6	2.30	1.36	1.32
2	C	601	1VU	O12-C22	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1VU	C20-N6	2.56	1.36	1.32
2	F	601	1VU	C20-N6	2.56	1.36	1.32
2	D	601	1VU	C20-N6	2.63	1.36	1.32
2	E	601	1VU	C20-N6	2.70	1.36	1.32
3	B	601	COA	C2A-N3A	2.70	1.36	1.32
2	H	601	1VU	C20-N6	2.70	1.36	1.32
2	G	601	1VU	O-C2	2.72	1.25	1.21
2	G	601	1VU	C20-N6	2.85	1.36	1.32
2	F	601	1VU	C19-N4	2.96	1.46	1.34
2	A	601	1VU	C19-N4	3.01	1.46	1.34
2	E	601	1VU	C19-N4	3.01	1.46	1.34
2	D	601	1VU	C19-N4	3.06	1.46	1.34
3	B	601	COA	C6A-N6A	3.07	1.46	1.34
2	C	601	1VU	C19-N4	3.09	1.46	1.34
2	H	601	1VU	C19-N4	3.13	1.46	1.34
2	G	601	1VU	C19-N4	3.17	1.47	1.34
2	E	601	1VU	C8-N1	4.82	1.43	1.33
2	A	601	1VU	C8-N1	5.19	1.44	1.33
2	F	601	1VU	C8-N1	5.20	1.44	1.33
3	B	601	COA	C9P-N8P	5.24	1.44	1.33
2	H	601	1VU	C8-N1	5.28	1.44	1.33
2	C	601	1VU	C8-N1	5.28	1.44	1.33
2	E	601	1VU	C5-N	5.31	1.45	1.33
2	A	601	1VU	C5-N	5.32	1.45	1.33
2	G	601	1VU	C13-C10	5.40	1.59	1.52
2	D	601	1VU	C8-N1	5.40	1.44	1.33
3	B	601	COA	C5P-N4P	5.41	1.46	1.33
2	G	601	1VU	C8-N1	5.44	1.44	1.33
2	F	601	1VU	C5-N	5.53	1.46	1.33
2	D	601	1VU	C5-N	5.54	1.46	1.33
2	G	601	1VU	C5-N	5.56	1.46	1.33
2	C	601	1VU	C5-N	5.58	1.46	1.33
2	H	601	1VU	C5-N	5.69	1.46	1.33
2	A	601	1VU	C13-C10	6.07	1.60	1.52
2	C	601	1VU	C13-C10	6.19	1.60	1.52
2	D	601	1VU	C13-C10	6.26	1.60	1.52
2	E	601	1VU	C13-C10	6.34	1.61	1.52
3	B	601	COA	CCP-CBP	6.38	1.61	1.52
2	H	601	1VU	C13-C10	6.45	1.61	1.52
2	F	601	1VU	C13-C10	6.60	1.61	1.52
2	C	601	1VU	O11-C16	13.55	1.60	1.41
2	E	601	1VU	O11-C16	13.70	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	1VU	O11-C16	13.70	1.60	1.41
2	H	601	1VU	O11-C16	13.74	1.60	1.41
2	F	601	1VU	O11-C16	13.81	1.60	1.41
3	B	601	COA	O4B-C1B	13.91	1.60	1.41
2	D	601	1VU	O11-C16	14.09	1.60	1.41
2	A	601	1VU	O11-C16	14.28	1.61	1.41

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	1VU	N6-C20-N5	-10.42	119.78	128.86
2	F	601	1VU	N6-C20-N5	-10.28	119.90	128.86
2	C	601	1VU	N6-C20-N5	-10.13	120.03	128.86
2	G	601	1VU	N6-C20-N5	-10.11	120.05	128.86
2	A	601	1VU	N6-C20-N5	-10.10	120.06	128.86
2	H	601	1VU	N6-C20-N5	-10.07	120.09	128.86
3	B	601	COA	N3A-C2A-N1A	-9.99	120.16	128.86
2	D	601	1VU	N6-C20-N5	-9.54	120.55	128.86
2	G	601	1VU	C11-C10-C13	-6.10	99.41	108.37
2	H	601	1VU	O-C2-S	-5.42	117.16	122.84
2	F	601	1VU	O-C2-C1	-4.99	117.01	123.50
2	H	601	1VU	C15-O11-C16	-4.99	104.46	109.77
2	C	601	1VU	O-C2-S	-4.84	117.77	122.84
2	F	601	1VU	C16-N2-C21	-4.26	119.27	126.64
2	D	601	1VU	C16-N2-C21	-4.02	119.68	126.64
2	C	601	1VU	C16-N2-C21	-3.80	120.07	126.64
2	H	601	1VU	C-C1-C2	-3.69	104.36	114.59
2	F	601	1VU	C15-O11-C16	-3.45	106.10	109.77
2	E	601	1VU	C15-O11-C16	-3.33	106.22	109.77
2	G	601	1VU	O-C2-C1	-3.29	119.22	123.50
2	E	601	1VU	O-C2-C1	-3.29	119.22	123.50
2	H	601	1VU	C16-N2-C21	-3.26	121.00	126.64
2	E	601	1VU	C16-N2-C21	-3.12	121.24	126.64
2	C	601	1VU	O-C2-C1	-3.02	119.56	123.50
2	A	601	1VU	C16-N2-C21	-2.95	121.53	126.64
2	H	601	1VU	O-C2-C1	-2.87	119.76	123.50
2	G	601	1VU	C16-N2-C21	-2.87	121.68	126.64
2	D	601	1VU	O-C2-C1	-2.77	119.89	123.50
2	G	601	1VU	O2-C8-N1	-2.75	117.78	123.07
2	A	601	1VU	O-C2-S	-2.73	119.98	122.84
2	F	601	1VU	O-C2-S	-2.70	120.02	122.84
2	E	601	1VU	C4-N-C5	-2.69	117.67	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	COA	C1B-N9A-C4A	-2.69	121.99	126.64
2	A	601	1VU	O-C2-C1	-2.63	120.08	123.50
2	E	601	1VU	O-C2-S	-2.61	120.11	122.84
2	E	601	1VU	C7-C6-C5	-2.52	108.16	112.22
2	G	601	1VU	C15-O11-C16	-2.52	107.08	109.77
2	E	601	1VU	C14-C15-C23	-2.51	105.78	114.30
2	A	601	1VU	C7-C6-C5	-2.48	108.24	112.22
2	E	601	1VU	C6-C7-N1	-2.40	106.89	111.87
2	G	601	1VU	P-O4-C13	-2.38	106.52	121.57
2	G	601	1VU	O4-P-O5	-2.33	99.84	109.25
2	E	601	1VU	C22-C23-C15	-2.25	99.21	103.23
2	D	601	1VU	C-C1-C2	-2.20	108.49	114.59
2	A	601	1VU	C-C1-C2	-2.13	108.69	114.59
2	C	601	1VU	C7-C6-C5	-2.11	108.82	112.22
2	H	601	1VU	O2-C8-N1	-2.09	119.05	123.07
2	D	601	1VU	C7-C6-C5	-2.03	108.96	112.22
2	A	601	1VU	O2-C8-N1	-2.02	119.17	123.07
3	B	601	COA	C6P-C7P-N8P	-2.01	107.71	111.87
2	G	601	1VU	C11-C10-C9	2.10	112.46	108.82
2	E	601	1VU	C6-C5-N	2.10	120.12	116.49
2	A	601	1VU	C6-C5-N	2.11	120.13	116.49
2	E	601	1VU	C3-S-C2	2.23	109.29	101.90
2	F	601	1VU	C23-C22-C16	2.27	105.04	99.95
2	C	601	1VU	C3-S-C2	2.32	109.57	101.90
2	H	601	1VU	C6-C5-N	2.37	120.58	116.49
2	D	601	1VU	C6-C5-N	2.41	120.64	116.49
2	H	601	1VU	C23-C22-C16	2.55	105.68	99.95
2	C	601	1VU	C23-C22-C16	2.56	105.70	99.95
2	G	601	1VU	C6-C5-N	2.56	120.91	116.49
3	B	601	COA	C6P-C5P-N4P	2.66	121.08	116.49
2	G	601	1VU	C3-S-C2	3.12	112.23	101.90
2	H	601	1VU	C3-S-C2	3.14	112.28	101.90
2	A	601	1VU	C3-S-C2	3.15	112.31	101.90
2	D	601	1VU	C3-S-C2	3.23	112.58	101.90
2	F	601	1VU	C3-S-C2	3.39	113.11	101.90
2	G	601	1VU	C23-C22-C16	3.40	107.58	99.95
2	G	601	1VU	C9-C8-N1	3.62	124.11	116.58
2	D	601	1VU	C1-C2-S	4.70	117.99	113.31
2	G	601	1VU	C1-C2-S	6.09	119.39	113.31
2	A	601	1VU	C1-C2-S	6.65	119.94	113.31
2	E	601	1VU	C1-C2-S	7.37	120.67	113.31
2	C	601	1VU	C1-C2-S	9.36	122.65	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	1VU	C1-C2-S	9.69	122.97	113.31
2	H	601	1VU	C1-C2-S	9.72	123.01	113.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	1VU	C1-C2-S-C3
2	F	601	1VU	O-C2-S-C3
2	G	601	1VU	O-C2-C1-C
2	D	601	1VU	C9-C8-N1-C7
2	G	601	1VU	C9-C8-N1-C7

There are no ring outliers.

8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	1VU	6	0
3	B	601	COA	1	0
2	C	601	1VU	5	0
2	D	601	1VU	5	0
2	E	601	1VU	8	0
2	F	601	1VU	4	0
2	G	601	1VU	3	0
2	H	601	1VU	8	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	439/524 (83%)	-0.54	6 (1%) 75 77	22, 32, 54, 85	0
1	B	452/524 (86%)	-0.55	5 (1%) 80 82	22, 31, 52, 83	0
1	C	439/524 (83%)	-0.60	1 (0%) 94 95	22, 32, 48, 65	0
1	D	439/524 (83%)	-0.26	6 (1%) 75 77	25, 37, 62, 81	0
1	E	439/524 (83%)	-0.53	6 (1%) 75 77	22, 33, 54, 76	0
1	F	452/524 (86%)	-0.51	8 (1%) 69 71	21, 32, 62, 84	0
1	G	439/524 (83%)	-0.43	8 (1%) 69 71	22, 38, 63, 88	0
1	H	441/524 (84%)	-0.31	7 (1%) 72 74	24, 40, 64, 78	0
All	All	3540/4192 (84%)	-0.47	47 (1%) 77 79	21, 34, 59, 88	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	LYS	5.5
1	A	376	GLY	5.4
1	B	53	ALA	5.0
1	A	374	ALA	4.1
1	E	375	LYS	4.1
1	B	54	ASP	4.0
1	D	374	ALA	3.9
1	G	375	LYS	3.8
1	F	53	ALA	3.8
1	F	362	ALA	3.7
1	G	376	GLY	3.7
1	H	84	ALA	3.7
1	D	86	VAL	3.7
1	G	374	ALA	3.6
1	E	376	GLY	3.6
1	B	52	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	374	ALA	3.5
1	G	362	ALA	3.4
1	F	51	SER	3.2
1	B	50	ASN	3.1
1	F	50	ASN	2.9
1	F	375	LYS	2.8
1	H	398	VAL	2.7
1	A	400	ALA	2.7
1	D	375	LYS	2.7
1	H	86	VAL	2.7
1	F	52	SER	2.6
1	H	374	ALA	2.6
1	G	373	THR	2.6
1	A	259	ILE	2.6
1	B	51	SER	2.6
1	G	361	PRO	2.6
1	H	376	GLY	2.6
1	F	361	PRO	2.5
1	F	376	GLY	2.5
1	H	242	ALA	2.4
1	D	394	ILE	2.4
1	C	86	VAL	2.4
1	D	376	GLY	2.3
1	E	400	ALA	2.3
1	E	397	SER	2.3
1	G	369	ASP	2.2
1	H	400	ALA	2.2
1	E	259	ILE	2.2
1	D	373	THR	2.1
1	G	364	LEU	2.1
1	A	260	GLU	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
2	1VU	G	601	52/52	0.71	0.29	4.57	49,76,91,95	52
2	1VU	C	601	52/52	0.76	0.23	2.25	33,61,77,93	52
3	COA	B	601	48/48	0.82	0.21	2.04	39,61,76,79	48
2	1VU	F	601	52/52	0.82	0.20	1.94	38,60,75,85	52
2	1VU	E	601	52/52	0.80	0.21	1.72	37,65,80,91	52
2	1VU	H	601	52/52	0.77	0.23	1.66	45,75,87,99	52
2	1VU	A	601	52/52	0.76	0.22	1.61	37,64,77,91	52
2	1VU	D	601	52/52	0.81	0.22	1.22	42,65,80,93	52

6.5 Other polymers [i](#)

There are no such residues in this entry.