WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 05:44 PM EST

PDB ID	:	5LOT
Title	:	Crystal structure of SCP2 thiolase from Leishmania mexicana. Complex of the C123A mutant with acetyl-CoA.
Authors	:	Harijan, R.K.; Kiema, T.-R.; Wierenga, R.K.
Deposited on	:	2016-08-09
Resolution	:	2.25 Å(reported)

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

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

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

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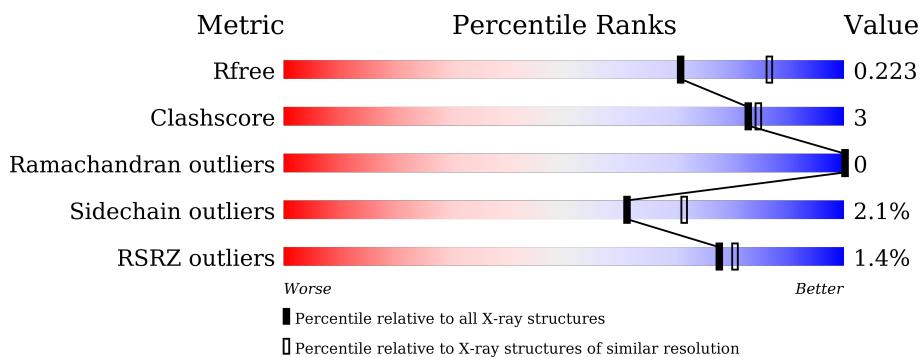
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
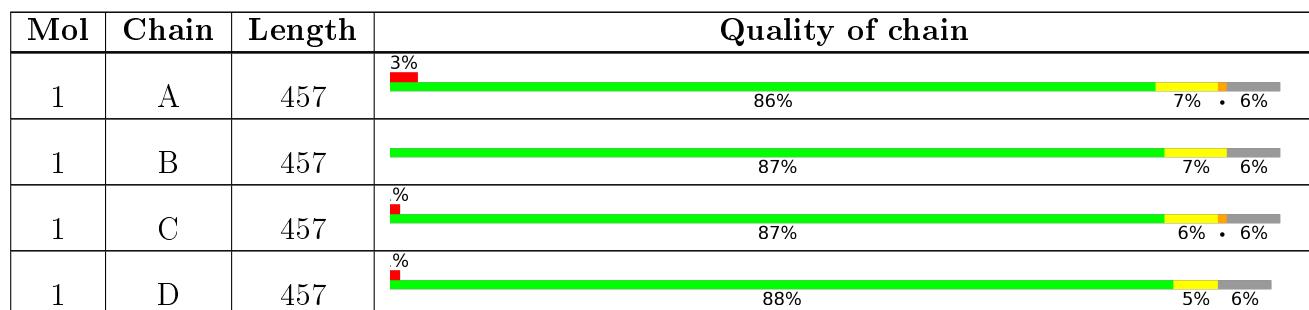
The reported resolution of this entry is 2.25 Å.

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	Percentile Ranks	Value
Rfree		0.223
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		1.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	457	3% 86% 7% · 6%
1	B	457	87% 7% 6%
1	C	457	% 87% 6% · 6%
1	D	457	% 88% 5% 6%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACO	A	501	-	-	-	X
2	ACO	D	501	-	-	-	X

Full wwPDB X-ray Structure Validation Report

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13679 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-ketoacyl-CoA thiolase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			
1	B	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			
1	C	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			
1	D	430	Total	C	N	O	S	0	0	0
			3223	2010	566	621	26			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP E9AW84
A	-14	HIS	-	expression tag	UNP E9AW84
A	-13	HIS	-	expression tag	UNP E9AW84
A	-12	HIS	-	expression tag	UNP E9AW84
A	-11	HIS	-	expression tag	UNP E9AW84
A	-10	HIS	-	expression tag	UNP E9AW84
A	-9	SER	-	expression tag	UNP E9AW84
A	-8	SER	-	expression tag	UNP E9AW84
A	-7	GLY	-	expression tag	UNP E9AW84
A	-6	LEU	-	expression tag	UNP E9AW84
A	-5	VAL	-	expression tag	UNP E9AW84
A	-4	PRO	-	expression tag	UNP E9AW84
A	-3	ARG	-	expression tag	UNP E9AW84
A	-2	GLY	-	expression tag	UNP E9AW84
A	-1	SER	-	expression tag	UNP E9AW84
A	0	HIS	-	expression tag	UNP E9AW84
A	6	LEU	MET	conflict	UNP E9AW84
A	12	ALA	THR	conflict	UNP E9AW84
A	31	PRO	LYS	conflict	UNP E9AW84
A	34	ILE	VAL	conflict	UNP E9AW84
A	45	LYS	GLN	conflict	UNP E9AW84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	HIS	conflict	UNP E9AW84
A	61	MET	ILE	conflict	UNP E9AW84
A	63	HIS	ASN	conflict	UNP E9AW84
A	64	SER	VAL	conflict	UNP E9AW84
A	65	GLY	SER	conflict	UNP E9AW84
A	67	SER	LYS	conflict	UNP E9AW84
A	69	ARG	LYS	conflict	UNP E9AW84
A	71	GLY	ASP	conflict	UNP E9AW84
A	107	SER	ALA	conflict	UNP E9AW84
A	112	MET	ILE	conflict	UNP E9AW84
A	123	ALA	CYS	conflict	UNP E9AW84
A	134	MET	THR	conflict	UNP E9AW84
A	139	SER	ALA	conflict	UNP E9AW84
A	145	THR	VAL	conflict	UNP E9AW84
A	157	SER	THR	conflict	UNP E9AW84
A	176	GLN	LYS	conflict	UNP E9AW84
A	229	THR	SER	conflict	UNP E9AW84
A	268	VAL	ALA	conflict	UNP E9AW84
A	277	ARG	LYS	conflict	UNP E9AW84
A	327	ILE	VAL	conflict	UNP E9AW84
A	356	GLU	ASP	conflict	UNP E9AW84
A	368	ASP	GLU	conflict	UNP E9AW84
A	398	ILE	VAL	conflict	UNP E9AW84
A	410	GLU	GLY	conflict	UNP E9AW84
B	-15	HIS	-	expression tag	UNP E9AW84
B	-14	HIS	-	expression tag	UNP E9AW84
B	-13	HIS	-	expression tag	UNP E9AW84
B	-12	HIS	-	expression tag	UNP E9AW84
B	-11	HIS	-	expression tag	UNP E9AW84
B	-10	HIS	-	expression tag	UNP E9AW84
B	-9	SER	-	expression tag	UNP E9AW84
B	-8	SER	-	expression tag	UNP E9AW84
B	-7	GLY	-	expression tag	UNP E9AW84
B	-6	LEU	-	expression tag	UNP E9AW84
B	-5	VAL	-	expression tag	UNP E9AW84
B	-4	PRO	-	expression tag	UNP E9AW84
B	-3	ARG	-	expression tag	UNP E9AW84
B	-2	GLY	-	expression tag	UNP E9AW84
B	-1	SER	-	expression tag	UNP E9AW84
B	0	HIS	-	expression tag	UNP E9AW84
B	6	LEU	MET	conflict	UNP E9AW84
B	12	ALA	THR	conflict	UNP E9AW84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	PRO	LYS	conflict	UNP E9AW84
B	34	ILE	VAL	conflict	UNP E9AW84
B	45	LYS	GLN	conflict	UNP E9AW84
B	59	GLY	HIS	conflict	UNP E9AW84
B	61	MET	ILE	conflict	UNP E9AW84
B	63	HIS	ASN	conflict	UNP E9AW84
B	64	SER	VAL	conflict	UNP E9AW84
B	65	GLY	SER	conflict	UNP E9AW84
B	67	SER	LYS	conflict	UNP E9AW84
B	69	ARG	LYS	conflict	UNP E9AW84
B	71	GLY	ASP	conflict	UNP E9AW84
B	107	SER	ALA	conflict	UNP E9AW84
B	112	MET	ILE	conflict	UNP E9AW84
B	123	ALA	CYS	conflict	UNP E9AW84
B	134	MET	THR	conflict	UNP E9AW84
B	139	SER	ALA	conflict	UNP E9AW84
B	145	THR	VAL	conflict	UNP E9AW84
B	157	SER	THR	conflict	UNP E9AW84
B	176	GLN	LYS	conflict	UNP E9AW84
B	229	THR	SER	conflict	UNP E9AW84
B	268	VAL	ALA	conflict	UNP E9AW84
B	277	ARG	LYS	conflict	UNP E9AW84
B	327	ILE	VAL	conflict	UNP E9AW84
B	356	GLU	ASP	conflict	UNP E9AW84
B	368	ASP	GLU	conflict	UNP E9AW84
B	398	ILE	VAL	conflict	UNP E9AW84
B	410	GLU	GLY	conflict	UNP E9AW84
C	-15	HIS	-	expression tag	UNP E9AW84
C	-14	HIS	-	expression tag	UNP E9AW84
C	-13	HIS	-	expression tag	UNP E9AW84
C	-12	HIS	-	expression tag	UNP E9AW84
C	-11	HIS	-	expression tag	UNP E9AW84
C	-10	HIS	-	expression tag	UNP E9AW84
C	-9	SER	-	expression tag	UNP E9AW84
C	-8	SER	-	expression tag	UNP E9AW84
C	-7	GLY	-	expression tag	UNP E9AW84
C	-6	LEU	-	expression tag	UNP E9AW84
C	-5	VAL	-	expression tag	UNP E9AW84
C	-4	PRO	-	expression tag	UNP E9AW84
C	-3	ARG	-	expression tag	UNP E9AW84
C	-2	GLY	-	expression tag	UNP E9AW84
C	-1	SER	-	expression tag	UNP E9AW84

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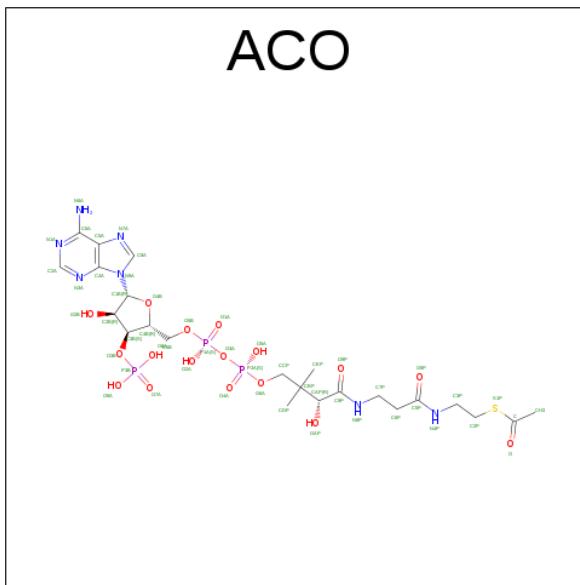
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP E9AW84
C	6	LEU	MET	conflict	UNP E9AW84
C	12	ALA	THR	conflict	UNP E9AW84
C	31	PRO	LYS	conflict	UNP E9AW84
C	34	ILE	VAL	conflict	UNP E9AW84
C	45	LYS	GLN	conflict	UNP E9AW84
C	59	GLY	HIS	conflict	UNP E9AW84
C	61	MET	ILE	conflict	UNP E9AW84
C	63	HIS	ASN	conflict	UNP E9AW84
C	64	SER	VAL	conflict	UNP E9AW84
C	65	GLY	SER	conflict	UNP E9AW84
C	67	SER	LYS	conflict	UNP E9AW84
C	69	ARG	LYS	conflict	UNP E9AW84
C	71	GLY	ASP	conflict	UNP E9AW84
C	107	SER	ALA	conflict	UNP E9AW84
C	112	MET	ILE	conflict	UNP E9AW84
C	123	ALA	CYS	conflict	UNP E9AW84
C	134	MET	THR	conflict	UNP E9AW84
C	139	SER	ALA	conflict	UNP E9AW84
C	145	THR	VAL	conflict	UNP E9AW84
C	157	SER	THR	conflict	UNP E9AW84
C	176	GLN	LYS	conflict	UNP E9AW84
C	229	THR	SER	conflict	UNP E9AW84
C	268	VAL	ALA	conflict	UNP E9AW84
C	277	ARG	LYS	conflict	UNP E9AW84
C	327	ILE	VAL	conflict	UNP E9AW84
C	356	GLU	ASP	conflict	UNP E9AW84
C	368	ASP	GLU	conflict	UNP E9AW84
C	398	ILE	VAL	conflict	UNP E9AW84
C	410	GLU	GLY	conflict	UNP E9AW84
D	-15	HIS	-	expression tag	UNP E9AW84
D	-14	HIS	-	expression tag	UNP E9AW84
D	-13	HIS	-	expression tag	UNP E9AW84
D	-12	HIS	-	expression tag	UNP E9AW84
D	-11	HIS	-	expression tag	UNP E9AW84
D	-10	HIS	-	expression tag	UNP E9AW84
D	-9	SER	-	expression tag	UNP E9AW84
D	-8	SER	-	expression tag	UNP E9AW84
D	-7	GLY	-	expression tag	UNP E9AW84
D	-6	LEU	-	expression tag	UNP E9AW84
D	-5	VAL	-	expression tag	UNP E9AW84
D	-4	PRO	-	expression tag	UNP E9AW84

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	ARG	-	expression tag	UNP E9AW84
D	-2	GLY	-	expression tag	UNP E9AW84
D	-1	SER	-	expression tag	UNP E9AW84
D	0	HIS	-	expression tag	UNP E9AW84
D	6	LEU	MET	conflict	UNP E9AW84
D	12	ALA	THR	conflict	UNP E9AW84
D	31	PRO	LYS	conflict	UNP E9AW84
D	34	ILE	VAL	conflict	UNP E9AW84
D	45	LYS	GLN	conflict	UNP E9AW84
D	59	GLY	HIS	conflict	UNP E9AW84
D	61	MET	ILE	conflict	UNP E9AW84
D	63	HIS	ASN	conflict	UNP E9AW84
D	64	SER	VAL	conflict	UNP E9AW84
D	65	GLY	SER	conflict	UNP E9AW84
D	67	SER	LYS	conflict	UNP E9AW84
D	69	ARG	LYS	conflict	UNP E9AW84
D	71	GLY	ASP	conflict	UNP E9AW84
D	107	SER	ALA	conflict	UNP E9AW84
D	112	MET	ILE	conflict	UNP E9AW84
D	123	ALA	CYS	conflict	UNP E9AW84
D	134	MET	THR	conflict	UNP E9AW84
D	139	SER	ALA	conflict	UNP E9AW84
D	145	THR	VAL	conflict	UNP E9AW84
D	157	SER	THR	conflict	UNP E9AW84
D	176	GLN	LYS	conflict	UNP E9AW84
D	229	THR	SER	conflict	UNP E9AW84
D	268	VAL	ALA	conflict	UNP E9AW84
D	277	ARG	LYS	conflict	UNP E9AW84
D	327	ILE	VAL	conflict	UNP E9AW84
D	356	GLU	ASP	conflict	UNP E9AW84
D	368	ASP	GLU	conflict	UNP E9AW84
D	398	ILE	VAL	conflict	UNP E9AW84
D	410	GLU	GLY	conflict	UNP E9AW84

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S		0	0
			51	23	7	17	3	1			
2	B	1	Total	C	N	O	P	S		0	0
			51	23	7	17	3	1			
2	D	1	Total	C	N	O	P	S		0	0
			51	23	7	17	3	1			
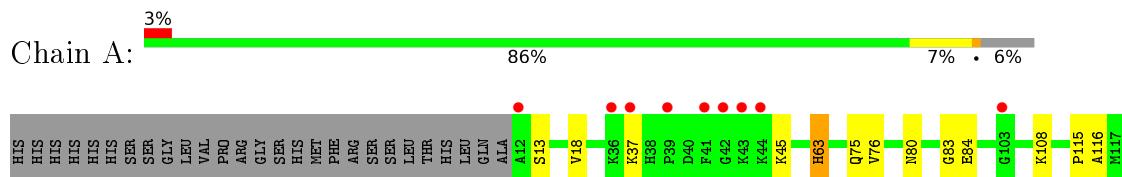
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	197	Total	O	0	0
			197	197		
3	C	151	Total	O	0	0
			151	151		
3	D	164	Total	O	0	0
			164	164		
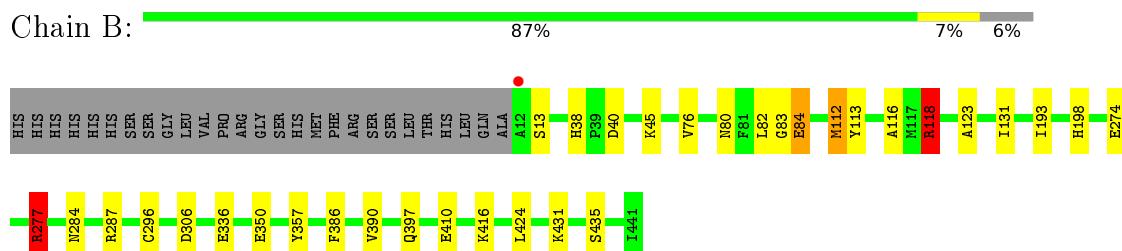
3 Residue-property plots ⓘ

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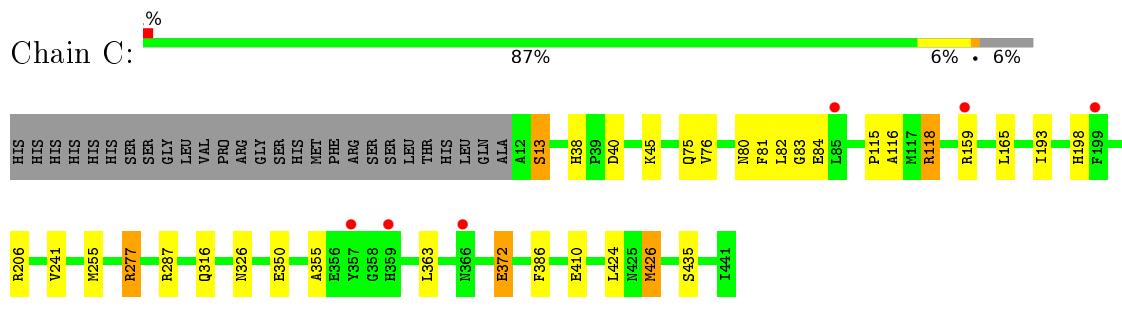
- Molecule 1: 3-ketoacyl-CoA thiolase-like protein
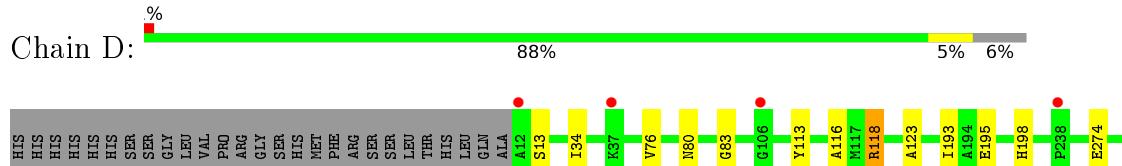
- Molecule 1: 3-ketoacyl-CoA thiolase-like protein

- Molecule 1: 3-ketoacyl-CoA thiolase-like protein

- Molecule 1: 3-ketoacyl-CoA thiolase-like protein

R277 N284 R287 Q319 K328 E336 E350 H359 R374 F386 V390 Q397 L424 S435 I441

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.70Å 89.89Å 126.33Å 90.00° 105.78° 90.00°	Depositor
Resolution (Å)	47.30 – 2.25 47.26 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.30-2.25) 98.2 (47.26-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.46 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.255 0.221 , 0.223	Depositor DCC
R_{free} test set	3952 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.6	EDS
L-test for twinning[2]	$<|L|>=0.51$, $<L^2>=0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13679	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACO

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	0.60	0/3276	0.73	3/4417 (0.1%)
1	B	0.69	2/3276 (0.1%)	0.78	7/4417 (0.2%)
1	C	0.64	1/3276 (0.0%)	0.75	4/4417 (0.1%)
1	D	0.61	0/3276	0.73	4/4417 (0.1%)
All	All	0.64	3/13104 (0.0%)	0.75	18/17668 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	GLU	CD-OE1	9.43	1.36	1.25
1	C	84	GLU	CD-OE2	5.05	1.31	1.25
1	B	84	GLU	CD-OE2	5.04	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	118	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	118	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	C	118	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	118	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	C	118	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	118	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	306	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	D	118	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	112	MET	CG-SD-CE	-5.98	90.64	100.20
1	C	426	MET	CB-CG-SD	-5.80	95.01	112.40
1	D	277	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	287	ARG	CG-CD-NE	-5.52	100.21	111.80
1	A	63	HIS	CB-CA-C	5.36	121.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	ARG	CG-CD-NE	-5.33	100.62	111.80
1	C	277	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	B	306	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	277	ARG	NE-CZ-NH2	5.01	122.80	120.30

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	3223	0	3202	25	0
1	B	3223	0	3202	20	0
1	C	3223	0	3202	21	0
1	D	3223	0	3202	14	0
2	A	51	0	34	3	0
2	B	51	0	34	1	0
2	D	51	0	34	3	0
3	A	122	0	0	5	0
3	B	197	0	0	6	0
3	C	151	0	0	6	0
3	D	164	0	0	6	0
All	All	13679	0	12910	80	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 3.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ILE:C	3:A:632:HOH:O	1.83	1.17
1:C:410:GLU:HG3	3:C:614:HOH:O	1.80	0.82
2:A:501:ACO:H8A	2:A:501:ACO:O5B	1.82	0.79
1:A:18:VAL:O	1:A:287:ARG:NH1	2.17	0.78
1:D:374:ARG:HD2	3:D:722:HOH:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:GLU:OE2	3:D:601:HOH:O	2.13	0.67
1:C:75:GLN:HG2	1:C:115:PRO:HB2	1.78	0.66
1:A:75:GLN:HG2	1:A:115:PRO:HB2	1.81	0.63
1:D:80:ASN:HD21	1:D:83:GLY:H	1.49	0.61
1:A:80:ASN:HD21	1:A:83:GLY:H	1.48	0.61
1:B:123:ALA:HA	1:B:390:VAL:HG13	1.83	0.61
1:D:123:ALA:HA	1:D:390:VAL:HG13	1.82	0.60
1:B:80:ASN:HD21	1:B:83:GLY:H	1.50	0.59
1:C:80:ASN:HD21	1:C:83:GLY:H	1.50	0.58
1:D:195:GLU:HG3	3:D:677:HOH:O	2.04	0.58
1:A:274:GLU:OE2	1:A:277:ARG:NH2	2.37	0.57
1:B:410:GLU:HG3	3:B:742:HOH:O	2.04	0.57
2:D:501:ACO:HH32	3:D:713:HOH:O	2.05	0.57
2:D:501:ACO:H131	2:D:501:ACO:O9P	2.04	0.57
1:A:37:LYS:HE3	3:A:702:HOH:O	2.05	0.56
1:B:84:GLU:CD	1:B:118:ARG:HH22	2.09	0.56
1:A:37:LYS:HG3	3:A:702:HOH:O	2.08	0.54
1:B:193:ILE:HG23	1:B:198:HIS:HB3	1.89	0.54
1:B:431:LYS:HE3	3:B:747:HOH:O	2.07	0.54
1:A:193:ILE:HG23	1:A:198:HIS:HB3	1.90	0.54
2:A:501:ACO:O9P	2:A:501:ACO:H141	2.08	0.53
1:A:176:GLN:HA	1:A:176:GLN:HE21	1.74	0.53
1:A:84:GLU:HG3	3:B:602:HOH:O	2.09	0.53
1:C:193:ILE:HG23	1:C:198:HIS:HB3	1.91	0.52
1:C:38:HIS:CE1	3:C:529:HOH:O	2.61	0.52
1:D:193:ILE:HG23	1:D:198:HIS:HB3	1.91	0.52
1:A:424:LEU:HD13	1:A:435:SER:HB2	1.92	0.51
1:B:274:GLU:OE2	1:B:277:ARG:NH2	2.44	0.51
1:C:372:GLU:OE2	1:C:372:GLU:HA	2.11	0.51
1:B:198:HIS:HD2	3:B:757:HOH:O	1.94	0.51
1:B:38:HIS:HD2	1:B:40:ASP:H	1.58	0.51
1:C:316:GLN:HG3	1:D:113:TYR:CG	2.46	0.50
1:A:18:VAL:HG12	1:A:287:ARG:NH1	2.27	0.49
2:B:501:ACO:HH32	3:B:721:HOH:O	2.10	0.49
1:D:274:GLU:OE2	1:D:277:ARG:NH2	2.45	0.49
1:A:159:ARG:HB2	3:A:686:HOH:O	2.10	0.49
2:D:501:ACO:O9P	2:D:501:ACO:CDP	2.61	0.49
1:C:165:LEU:HB3	3:C:575:HOH:O	2.13	0.48
1:A:372:GLU:HA	1:A:372:GLU:OE2	2.14	0.48
1:C:241:VAL:HG12	1:C:255:MET:SD	2.54	0.48
1:D:34:ILE:HD11	3:D:740:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LYS:HE3	1:C:287:ARG:HB2	1.95	0.47
1:C:424:LEU:HD13	1:C:435:SER:HB2	1.97	0.46
1:A:76:VAL:O	1:A:116:ALA:HA	2.16	0.46
1:D:76:VAL:O	1:D:116:ALA:HA	2.16	0.46
1:B:336:GLU:HG2	1:B:397:GLN:HA	1.97	0.45
1:D:424:LEU:HD13	1:D:435:SER:HB2	1.97	0.45
1:C:76:VAL:O	1:C:116:ALA:HA	2.16	0.45
1:B:416:LYS:HE2	3:B:786:HOH:O	2.17	0.45
1:B:424:LEU:HD13	1:B:435:SER:HB2	1.99	0.45
1:A:63:HIS:O	1:A:287:ARG:NH2	2.44	0.45
1:B:76:VAL:O	1:B:116:ALA:HA	2.17	0.45
1:A:316:GLN:HG3	1:B:113:TYR:CG	2.51	0.45
1:A:84:GLU:OE1	1:B:82:LEU:HD23	2.17	0.45
1:A:241:VAL:HG12	1:A:255:MET:SD	2.57	0.44
1:C:13:SER:CB	3:C:601:HOH:O	2.65	0.44
1:C:206:ARG:HG2	3:C:636:HOH:O	2.18	0.43
1:C:13:SER:HB3	3:C:601:HOH:O	2.18	0.43
1:A:108:LYS:HE3	1:C:287:ARG:CB	2.48	0.43
1:A:355:ALA:HB2	1:A:363:LEU:HD13	1.99	0.43
1:C:38:HIS:HD2	1:C:40:ASP:H	1.66	0.43
1:C:355:ALA:HB2	1:C:363:LEU:HD13	2.00	0.43
3:A:671:HOH:O	1:B:112:MET:HE1	2.18	0.43
1:B:38:HIS:CD2	1:B:40:ASP:H	2.35	0.43
1:D:198:HIS:HE1	1:D:350:GLU:OE1	2.02	0.43
1:D:336:GLU:HG2	1:D:397:GLN:HA	2.00	0.42
1:A:241:VAL:HG21	2:A:501:ACO:C2A	2.50	0.42
1:C:81:PHE:CG	1:C:82:LEU:HG	2.55	0.42
1:D:359:HIS:CE1	3:D:736:HOH:O	2.73	0.41
1:B:357:TYR:CD1	1:C:277:ARG:HD3	2.55	0.41
1:A:124:ALA:HA	1:A:425:ASN:OD1	2.21	0.41
1:B:198:HIS:HE1	1:B:350:GLU:OE1	2.03	0.41
1:C:198:HIS:HE1	1:C:350:GLU:OE1	2.03	0.41
1:A:198:HIS:HE1	1:A:350:GLU:OE1	2.03	0.41
1:B:131:ILE:CD1	1:B:296:CYS:HB2	2.51	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	428/457 (94%)	420 (98%)	8 (2%)	0	100	100
1	B	428/457 (94%)	418 (98%)	10 (2%)	0	100	100
1	C	428/457 (94%)	420 (98%)	8 (2%)	0	100	100
1	D	428/457 (94%)	419 (98%)	9 (2%)	0	100	100
All	All	1712/1828 (94%)	1677 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/362 (93%)	331 (98%)	7 (2%)	61	71
1	B	338/362 (93%)	332 (98%)	6 (2%)	66	77
1	C	338/362 (93%)	330 (98%)	8 (2%)	57	67
1	D	338/362 (93%)	331 (98%)	7 (2%)	61	71
All	All	1352/1448 (93%)	1324 (98%)	28 (2%)	61	71

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

Mol	Chain	Res	Type
1	A	13	SER
1	A	45	LYS

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Mol	Chain	Res	Type
1	A	118	ARG
1	A	176	GLN
1	A	292	LYS
1	A	372	GLU
1	A	386	PHE
1	B	13	SER
1	B	45	LYS
1	B	118	ARG
1	B	277	ARG
1	B	284	ASN
1	B	386	PHE
1	C	13	SER
1	C	45	LYS
1	C	118	ARG
1	C	159	ARG
1	C	326	ASN
1	C	372	GLU
1	C	386	PHE
1	C	426	MET
1	D	13	SER
1	D	118	ARG
1	D	277	ARG
1	D	284	ASN
1	D	319	GLN
1	D	328	LYS
1	D	386	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	176	GLN
1	A	196	HIS
1	A	198	HIS
1	A	216	ASN
1	B	38	HIS
1	B	58	GLN
1	B	80	ASN
1	B	198	HIS
1	B	216	ASN
1	B	316	GLN
1	B	319	GLN

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Mol	Chain	Res	Type
1	C	38	HIS
1	C	80	ASN
1	C	172	GLN
1	C	198	HIS
1	C	216	ASN
1	D	58	GLN
1	D	80	ASN
1	D	172	GLN
1	D	198	HIS
1	D	216	ASN
1	D	316	GLN
1	D	359	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	ACO	A	501	-	44,53,53	0.96	2 (4%)	54,79,79	1.94	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	ACO	B	501	-	44,53,53	1.00	2 (4%)	54,79,79	2.00	10 (18%)
2	ACO	D	501	-	44,53,53	0.87	1 (2%)	54,79,79	2.22	15 (27%)

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	ACO	A	501	-	-	0/47/67/67	0/3/3/3
2	ACO	B	501	-	-	0/47/67/67	0/3/3/3
2	ACO	D	501	-	-	3/47/67/67	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ACO	C2B-C3B	-2.87	1.46	1.53
2	A	501	ACO	P3B-O8A	-2.08	1.47	1.54
2	A	501	ACO	C5A-C4A	2.67	1.46	1.40
2	B	501	ACO	C5A-C4A	3.14	1.47	1.40
2	D	501	ACO	C5A-C4A	3.20	1.47	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	ACO	N3A-C2A-N1A	-9.42	121.47	128.87
2	A	501	ACO	N3A-C2A-N1A	-7.43	123.03	128.87
2	B	501	ACO	N3A-C2A-N1A	-7.16	123.25	128.87
2	B	501	ACO	C3P-C2P-S1P	-5.53	96.78	111.47
2	B	501	ACO	C1B-N9A-C4A	-5.12	121.09	126.81
2	B	501	ACO	C7P-C6P-C5P	-4.40	104.66	112.22
2	A	501	ACO	C1B-N9A-C4A	-4.37	121.92	126.81
2	B	501	ACO	C4B-O4B-C1B	-4.27	105.12	109.64
2	D	501	ACO	C2P-C3P-N4P	-3.72	104.97	112.43
2	A	501	ACO	OAP-CAP-C9P	-3.36	102.53	110.52
2	D	501	ACO	C1B-N9A-C4A	-3.33	123.09	126.81
2	A	501	ACO	O5P-C5P-C6P	-3.05	116.67	121.97
2	D	501	ACO	O5P-C5P-N4P	-2.90	117.19	122.96
2	D	501	ACO	O9P-C9P-N8P	-2.78	117.51	123.04
2	A	501	ACO	C2B-C1B-N9A	-2.58	106.55	113.47
2	B	501	ACO	O5P-C5P-C6P	-2.48	117.67	121.97

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	ACO	O5P-C5P-C6P	-2.22	118.11	121.97
2	A	501	ACO	P3B-O3B-C3B	-2.13	116.12	121.56
2	D	501	ACO	O9A-P3B-O3B	-2.08	100.41	106.62
2	D	501	ACO	CDP-CBP-CAP	2.07	112.95	109.17
2	D	501	ACO	C2A-N1A-C6A	2.09	122.50	118.77
2	D	501	ACO	O2A-P1A-O1A	2.13	123.63	112.56
2	B	501	ACO	C2A-N1A-C6A	2.14	122.59	118.77
2	B	501	ACO	C2P-C3P-N4P	2.16	116.76	112.43
2	A	501	ACO	C3P-N4P-C5P	2.25	127.25	122.79
2	B	501	ACO	O5A-P2A-O4A	2.38	124.92	112.56
2	A	501	ACO	C3B-C2B-C1B	2.44	105.38	100.06
2	A	501	ACO	C2P-C3P-N4P	2.53	117.50	112.43
2	A	501	ACO	C2A-N1A-C6A	2.63	123.46	118.77
2	A	501	ACO	C2P-S1P-C	2.71	119.08	102.48
2	D	501	ACO	CDP-CBP-CCP	2.93	112.30	108.50
2	B	501	ACO	O9A-P3B-O7A	3.06	120.62	110.63
2	D	501	ACO	CAP-C9P-N8P	3.31	124.11	116.31
2	D	501	ACO	C3P-N4P-C5P	3.54	129.81	122.79
2	D	501	ACO	C7P-N8P-C9P	4.02	130.68	122.62
2	A	501	ACO	C3P-C2P-S1P	4.03	122.19	111.47
2	D	501	ACO	C6P-C5P-N4P	4.72	124.67	116.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	ACO	CH3-C-S1P-C2P
2	D	501	ACO	O-C-S1P-C2P
2	D	501	ACO	CAP-C9P-N8P-C7P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ACO	3	0
2	B	501	ACO	1	0
2	D	501	ACO	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	430/457 (94%)	0.14	13 (3%)	54	58	15, 31, 59, 99	0
1	B	430/457 (94%)	-0.18	1 (0%)	95	96	12, 22, 42, 77	0
1	C	430/457 (94%)	0.11	6 (1%)	78	80	13, 28, 59, 90	0
1	D	430/457 (94%)	-0.07	4 (0%)	85	87	14, 26, 51, 89	0
All	All	1720/1828 (94%)	0.00	24 (1%)	78	80	12, 26, 54, 99	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	LYS	4.1
1	A	103	GLY	4.1
1	A	41	PHE	3.2
1	A	12	ALA	3.2
1	A	237	ASP	3.0
1	B	12	ALA	3.0
1	C	357	TYR	2.9
1	A	282	SER	2.8
1	C	366	ASN	2.8
1	A	44	LYS	2.7
1	D	106	GLY	2.6
1	A	42	GLY	2.6
1	A	236	GLU	2.4
1	A	39	PRO	2.4
1	D	12	ALA	2.4
1	A	36	LYS	2.4
1	C	159	ARG	2.4
1	C	199	PHE	2.3
1	A	284	ASN	2.3
1	A	43	LYS	2.2
1	C	85	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	238	PRO	2.1
1	C	359	HIS	2.1
1	D	37	LYS	2.1

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	ACO	A	501	51/51	0.70	0.35	5.68	42,97,126,131	0
2	ACO	D	501	51/51	0.85	0.20	2.69	45,64,78,83	0
2	ACO	B	501	51/51	0.96	0.11	-0.50	16,21,28,44	0

6.5 Other polymers (i)

There are no such residues in this entry.