



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2016 – 04:26 PM EST

PDB ID : 5H7X
Title : Crystal structure of the complex of Phosphopantetheine adenylyltransferase from *Acinetobacter baumannii* with 2-hydroxy-1,2,3-propane tricarboxylate at 1.76 Å resolution
Authors : Singh, P.K.; Gupta, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-11-21
Resolution : 1.76 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-20028320
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-20028320

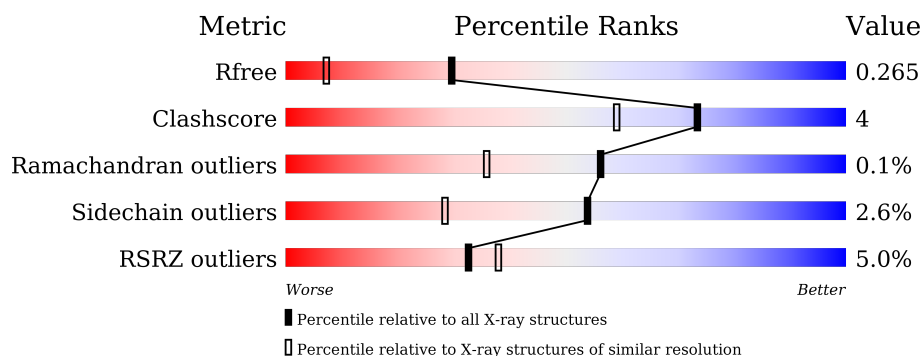
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	171	
1	B	171	
1	C	171	
1	D	171	
1	E	171	
1	F	171	

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	CIT	B	201	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8653 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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1305	838	227	237	3			
1	B	163	Total	C	N	O	S	0	0	0
			1305	838	227	237	3			
1	C	163	Total	C	N	O	S	0	0	0
			1305	838	227	237	3			
1	D	163	Total	C	N	O	S	0	0	0
			1305	838	227	237	3			
1	E	171	Total	C	N	O	S	0	0	0
			1362	873	240	246	3			
1	F	171	Total	C	N	O	S	0	0	0
			1362	873	240	246	3			

There are 48 discrepancies between the modelled and reference sequences:

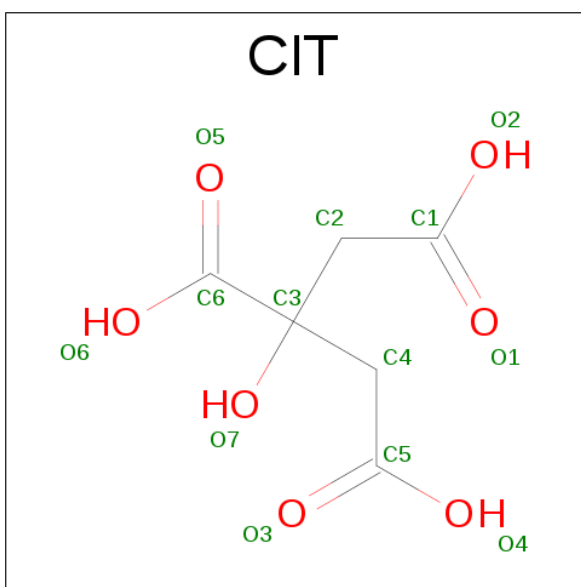
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A059ZFC5
A	-6	LEU	-	expression tag	UNP A0A059ZFC5
A	-5	VAL	-	expression tag	UNP A0A059ZFC5
A	-4	PRO	-	expression tag	UNP A0A059ZFC5
A	-3	ARG	-	expression tag	UNP A0A059ZFC5
A	-2	GLY	-	expression tag	UNP A0A059ZFC5
A	-1	SER	-	expression tag	UNP A0A059ZFC5
A	0	HIS	-	expression tag	UNP A0A059ZFC5
B	-7	GLY	-	expression tag	UNP A0A059ZFC5
B	-6	LEU	-	expression tag	UNP A0A059ZFC5
B	-5	VAL	-	expression tag	UNP A0A059ZFC5
B	-4	PRO	-	expression tag	UNP A0A059ZFC5
B	-3	ARG	-	expression tag	UNP A0A059ZFC5
B	-2	GLY	-	expression tag	UNP A0A059ZFC5
B	-1	SER	-	expression tag	UNP A0A059ZFC5
B	0	HIS	-	expression tag	UNP A0A059ZFC5
C	-7	GLY	-	expression tag	UNP A0A059ZFC5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	expression tag	UNP A0A059ZFC5
C	-5	VAL	-	expression tag	UNP A0A059ZFC5
C	-4	PRO	-	expression tag	UNP A0A059ZFC5
C	-3	ARG	-	expression tag	UNP A0A059ZFC5
C	-2	GLY	-	expression tag	UNP A0A059ZFC5
C	-1	SER	-	expression tag	UNP A0A059ZFC5
C	0	HIS	-	expression tag	UNP A0A059ZFC5
D	-7	GLY	-	expression tag	UNP A0A059ZFC5
D	-6	LEU	-	expression tag	UNP A0A059ZFC5
D	-5	VAL	-	expression tag	UNP A0A059ZFC5
D	-4	PRO	-	expression tag	UNP A0A059ZFC5
D	-3	ARG	-	expression tag	UNP A0A059ZFC5
D	-2	GLY	-	expression tag	UNP A0A059ZFC5
D	-1	SER	-	expression tag	UNP A0A059ZFC5
D	0	HIS	-	expression tag	UNP A0A059ZFC5
E	-7	GLY	-	expression tag	UNP A0A059ZFC5
E	-6	LEU	-	expression tag	UNP A0A059ZFC5
E	-5	VAL	-	expression tag	UNP A0A059ZFC5
E	-4	PRO	-	expression tag	UNP A0A059ZFC5
E	-3	ARG	-	expression tag	UNP A0A059ZFC5
E	-2	GLY	-	expression tag	UNP A0A059ZFC5
E	-1	SER	-	expression tag	UNP A0A059ZFC5
E	0	HIS	-	expression tag	UNP A0A059ZFC5
F	-7	GLY	-	expression tag	UNP A0A059ZFC5
F	-6	LEU	-	expression tag	UNP A0A059ZFC5
F	-5	VAL	-	expression tag	UNP A0A059ZFC5
F	-4	PRO	-	expression tag	UNP A0A059ZFC5
F	-3	ARG	-	expression tag	UNP A0A059ZFC5
F	-2	GLY	-	expression tag	UNP A0A059ZFC5
F	-1	SER	-	expression tag	UNP A0A059ZFC5
F	0	HIS	-	expression tag	UNP A0A059ZFC5

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

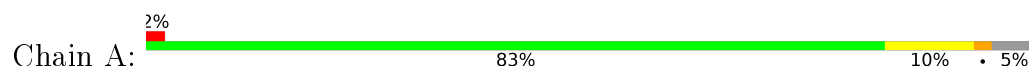
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	71	Total	O	0	0
			71	71		
3	C	98	Total	O	0	0
			98	98		
3	D	100	Total	O	0	0
			100	100		
3	E	108	Total	O	0	0
			108	108		
3	F	132	Total	O	0	0
			132	132		

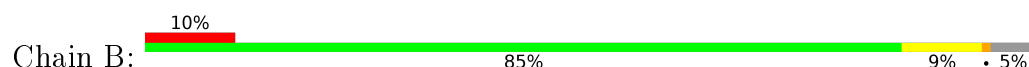
3 Residue-property plots [i](#)

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

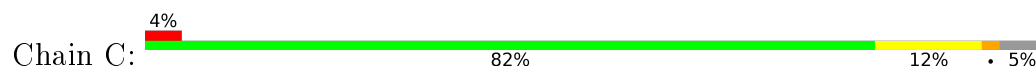
- Molecule 1: Phosphopantetheine adenylyltransferase



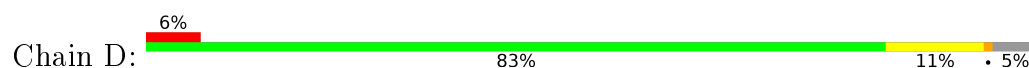
- Molecule 1: Phosphopantetheine adenylyltransferase



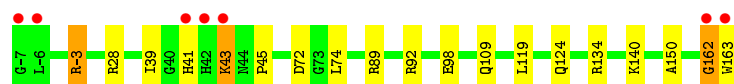
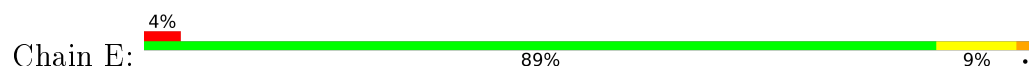
- Molecule 1: Phosphopantetheine adenylyltransferase



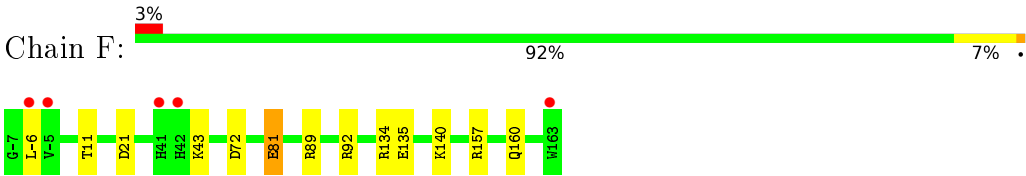
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.26Å 109.39Å 121.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.61 – 1.76 40.61 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.61-1.76) 99.6 (40.61-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.209 , 0.256 0.217 , 0.265	Depositor DCC
R_{free} test set	1118 reflections (1.09%)	DCC
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8653	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.18% 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: CIT

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	0.88	0/1335	1.00	7/1806 (0.4%)
1	B	0.77	0/1335	0.94	6/1806 (0.3%)
1	C	0.82	1/1335 (0.1%)	0.96	4/1806 (0.2%)
1	D	0.81	0/1335	0.96	7/1806 (0.4%)
1	E	0.83	0/1394	0.95	7/1886 (0.4%)
1	F	0.87	1/1394 (0.1%)	0.98	4/1886 (0.2%)
All	All	0.83	2/8128 (0.0%)	0.96	35/10996 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	81	GLU	CG-CD	5.86	1.60	1.51
1	C	98	GLU	CD-OE2	5.07	1.31	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	B	42	HIS	CB-CA-C	7.06	124.51	110.40
1	C	138	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	F	72	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	C	134	ARG	NE-CZ-NH2	-6.83	116.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	F	21	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	F	134	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	72	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	28	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	E	-3	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	50	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	B	89	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	162	GLY	N-CA-C	-5.83	98.51	113.10
1	A	52	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	E	89	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	106	MET	CG-SD-CE	5.58	109.12	100.20
1	A	28	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	1	MET	CA-CB-CG	5.54	122.71	113.30
1	B	72	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	28	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	92	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	B	31	ASP	CB-CG-OD1	5.28	123.05	118.30
1	E	98	GLU	N-CA-CB	-5.26	101.14	110.60
1	D	134	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	108	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	89	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	162	GLY	N-CA-C	5.17	126.01	113.10
1	B	28	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	76	VAL	CG1-CB-CG2	5.07	119.00	110.90
1	E	134	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	89	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	25	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	E	-3	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	74	LEU	CB-CG-CD1	5.02	119.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	162	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1305	0	1295	14	0
1	B	1305	0	1295	11	0
1	C	1305	0	1295	19	0
1	D	1305	0	1295	15	0
1	E	1362	0	1353	12	0
1	F	1362	0	1353	7	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	1	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	1	0
3	A	122	0	0	3	0
3	B	71	0	0	2	0
3	C	98	0	0	4	0
3	D	100	0	0	2	0
3	E	108	0	0	1	0
3	F	132	0	0	4	0
All	All	8653	0	7916	65	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 4.

All (65) 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:42:HIS:CE1	1:C:43:LYS:HG3	1.90	1.05
1:E:43:LYS:CA	1:E:43:LYS:HE3	2.15	0.77
1:C:42:HIS:CE1	1:C:43:LYS:CG	2.70	0.73
1:E:43:LYS:HE3	1:E:43:LYS:HA	1.72	0.71
1:E:43:LYS:C	1:E:43:LYS:HE3	2.11	0.71
1:C:42:HIS:O	1:C:43:LYS:C	2.29	0.69
1:B:113:HIS:ND1	3:B:301:HOH:O	2.26	0.67
1:D:106:MET:CE	1:D:110:LEU:HD12	2.27	0.65
1:C:42:HIS:ND1	1:C:43:LYS:HG3	2.14	0.63
1:A:94:VAL:HG22	1:B:98:GLU:OE2	1.99	0.63
1:A:139:LEU:HB2	1:B:74:LEU:HD13	1.81	0.62
2:C:201:CIT:O1	3:C:301:HOH:O	2.16	0.60
1:D:106:MET:CE	1:D:110:LEU:CD1	2.81	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:HA	3:A:390:HOH:O	2.02	0.59
1:E:43:LYS:O	1:E:43:LYS:HD3	2.05	0.57
1:D:106:MET:HE1	1:D:110:LEU:HD12	1.86	0.57
1:F:11:THR:HG21	1:F:43:LYS:CE	2.36	0.56
1:F:92:ARG:NH2	3:F:303:HOH:O	2.33	0.56
1:A:65:ASN:HB3	1:F:-6:LEU:HD11	1.88	0.55
1:C:42:HIS:CE1	1:C:43:LYS:CD	2.91	0.54
1:D:106:MET:HE3	1:D:110:LEU:CD1	2.38	0.53
1:E:41:HIS:ND1	1:E:41:HIS:O	2.41	0.53
1:C:92:ARG:NE	3:C:304:HOH:O	2.42	0.53
1:D:127:PHE:CZ	1:E:109:GLN:HG3	2.44	0.52
1:E:162:GLY:O	1:E:163:TRP:C	2.47	0.52
1:D:92:ARG:HD2	1:D:126:SER:O	2.08	0.52
1:D:106:MET:HE1	1:D:110:LEU:CD1	2.41	0.51
1:A:28:ARG:HD2	3:A:312:HOH:O	2.12	0.50
1:B:42:HIS:O	1:B:43:LYS:C	2.49	0.50
1:E:41:HIS:CG	1:E:41:HIS:O	2.66	0.49
1:A:135:GLU:HG2	3:B:370:HOH:O	2.13	0.49
1:F:135:GLU:HG2	3:F:398:HOH:O	2.14	0.48
1:A:74:LEU:HD21	1:C:141:GLY:HA2	1.95	0.48
1:C:51:GLU:HG2	3:C:366:HOH:O	2.13	0.47
1:F:11:THR:HG21	1:F:43:LYS:HE3	1.96	0.47
1:F:81:GLU:HG3	3:F:341:HOH:O	2.15	0.47
1:C:108:ARG:HD2	3:D:301:HOH:O	2.14	0.47
1:A:80:LYS:HD3	3:A:353:HOH:O	2.15	0.47
1:A:42:HIS:O	1:A:43:LYS:HB3	2.15	0.46
1:B:136:ILE:HA	1:C:74:LEU:HD21	1.96	0.46
1:E:43:LYS:CE	1:E:43:LYS:HA	2.44	0.46
1:A:106:MET:HB2	1:C:127:PHE:CD1	2.51	0.45
1:C:119:LEU:HD21	1:D:117:VAL:HG12	1.99	0.45
1:D:106:MET:HE2	1:D:107:ASN:N	2.32	0.44
1:B:117:VAL:HG12	1:E:119:LEU:HD21	1.98	0.44
1:B:127:PHE:HA	1:C:102:GLN:HG3	1.99	0.43
1:B:127:PHE:CZ	1:C:109:GLN:HG3	2.53	0.43
1:A:140:LYS:HE3	1:A:159:HIS:ND1	2.33	0.43
1:B:157:ARG:O	1:B:160:GLN:HG2	2.19	0.43
1:C:117:VAL:HG12	1:D:119:LEU:HD21	2.01	0.43
2:F:201:CIT:O3	3:F:301:HOH:O	2.21	0.43
1:C:119:LEU:CD2	1:D:117:VAL:HG12	2.49	0.42
1:B:43:LYS:HG3	1:B:43:LYS:O	2.19	0.42
1:A:42:HIS:O	1:A:43:LYS:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASN:HA	1:A:45:PRO:HD3	1.76	0.42
1:E:150:ALA:HB3	3:E:320:HOH:O	2.18	0.42
1:D:163:TRP:HB2	3:D:397:HOH:O	2.19	0.42
1:F:157:ARG:O	1:F:160:GLN:HG2	2.19	0.42
1:D:88:LEU:HD11	1:D:119:LEU:HG	2.03	0.41
1:D:157:ARG:O	1:D:160:GLN:HG2	2.20	0.41
1:C:29:MET:CE	1:D:117:VAL:HG11	2.51	0.41
1:C:44:ASN:OD1	1:C:45:PRO:N	2.53	0.41
1:C:98:GLU:OE1	3:C:302:HOH:O	2.22	0.40
1:E:43:LYS:C	1:E:43:LYS:CE	2.86	0.40
1:A:127:PHE:CZ	1:B:109:GLN:HG3	2.57	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	161/171 (94%)	159 (99%)	2 (1%)	0	100	100
1	B	161/171 (94%)	154 (96%)	7 (4%)	0	100	100
1	C	161/171 (94%)	155 (96%)	6 (4%)	0	100	100
1	D	161/171 (94%)	157 (98%)	4 (2%)	0	100	100
1	E	169/171 (99%)	164 (97%)	4 (2%)	1 (1%)	30	12
1	F	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
All	All	982/1026 (96%)	952 (97%)	29 (3%)	1 (0%)	56	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	162	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	141/147 (96%)	139 (99%)	2 (1%)	74	58
1	B	141/147 (96%)	138 (98%)	3 (2%)	61	37
1	C	141/147 (96%)	136 (96%)	5 (4%)	43	17
1	D	141/147 (96%)	138 (98%)	3 (2%)	61	37
1	E	147/147 (100%)	139 (95%)	8 (5%)	27	7
1	F	147/147 (100%)	146 (99%)	1 (1%)	88	79
All	All	858/882 (97%)	836 (97%)	22 (3%)	54	28

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	80	LYS
1	B	74	LEU
1	B	80	LYS
1	B	140	LYS
1	C	3	LYS
1	C	42	HIS
1	C	80	LYS
1	C	138	ARG
1	C	140	LYS
1	D	1	MET
1	D	43	LYS
1	D	140	LYS
1	E	-3	ARG
1	E	39	ILE
1	E	43	LYS
1	E	45	PRO
1	E	74	LEU
1	E	92	ARG
1	E	124	GLN
1	E	140	LYS
1	F	140	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	GLN
1	C	102	GLN
1	C	160	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](#)

6 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	CIT	A	201	-	3,12,12	3.05	1 (33%)	3,17,17	5.68	2 (66%)
2	CIT	B	201	-	3,12,12	0.19	0	3,17,17	4.35	2 (66%)
2	CIT	C	201	-	3,12,12	0.89	0	3,17,17	3.46	1 (33%)
2	CIT	D	201	-	3,12,12	1.11	0	3,17,17	7.15	3 (100%)
2	CIT	E	201	-	3,12,12	0.87	0	3,17,17	2.60	1 (33%)
2	CIT	F	201	-	3,12,12	1.62	1 (33%)	3,17,17	5.82	2 (66%)

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	CIT	A	201	-	-	0/6/16/16	0/0/0/0
2	CIT	B	201	-	-	0/6/16/16	0/0/0/0
2	CIT	C	201	-	-	0/6/16/16	0/0/0/0
2	CIT	D	201	-	-	0/6/16/16	0/0/0/0
2	CIT	E	201	-	-	0/6/16/16	0/0/0/0
2	CIT	F	201	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	CIT	C4-C3	-5.23	1.46	1.54
2	F	201	CIT	C4-C3	-2.48	1.50	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	CIT	C3-C4-C5	-10.76	98.14	114.95
2	A	201	CIT	C3-C4-C5	-7.09	103.87	114.95
2	F	201	CIT	C3-C4-C5	-6.11	105.41	114.95
2	B	201	CIT	C3-C4-C5	-6.00	105.57	114.95
2	C	201	CIT	C3-C2-C1	-5.78	105.91	114.95
2	E	201	CIT	C3-C2-C1	-4.44	108.01	114.95
2	D	201	CIT	C3-C2-C1	2.71	119.18	114.95
2	B	201	CIT	C3-C2-C1	4.30	121.66	114.95
2	D	201	CIT	C4-C3-C2	5.48	123.45	109.85
2	A	201	CIT	C4-C3-C2	6.80	126.73	109.85
2	F	201	CIT	C4-C3-C2	7.99	129.67	109.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	CIT	1	0
2	F	201	CIT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	163/171 (95%)	-0.02	4 (2%) 61 67	20, 30, 54, 93	0
1	B	163/171 (95%)	0.50	17 (10%) 8 11	23, 37, 90, 137	0
1	C	163/171 (95%)	0.19	7 (4%) 39 45	24, 35, 62, 120	0
1	D	163/171 (95%)	0.20	10 (6%) 25 29	24, 36, 79, 122	0
1	E	171/171 (100%)	0.17	7 (4%) 41 47	23, 34, 59, 165	0
1	F	171/171 (100%)	0.13	5 (2%) 55 61	20, 32, 75, 136	0
All	All	994/1026 (96%)	0.19	50 (5%) 32 38	20, 34, 76, 165	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	42	HIS	10.5
1	B	162	GLY	9.5
1	B	42	HIS	9.0
1	F	41	HIS	8.8
1	E	41	HIS	8.5
1	A	43	LYS	7.5
1	D	163	TRP	7.1
1	C	1	MET	6.4
1	B	163	TRP	6.3
1	C	42	HIS	6.0
1	E	42	HIS	6.0
1	E	-7	GLY	5.9
1	B	1	MET	5.4
1	C	43	LYS	5.4
1	E	43	LYS	5.1
1	B	41	HIS	5.0
1	D	42	HIS	4.8
1	B	45	PRO	4.7
1	C	2	SER	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	41	HIS	4.5
1	D	1	MET	4.4
1	C	41	HIS	4.4
1	D	2	SER	4.3
1	B	160	GLN	3.9
1	B	157	ARG	3.8
1	B	43	LYS	3.6
1	D	162	GLY	3.6
1	E	163	TRP	3.6
1	B	159	HIS	3.4
1	A	1	MET	3.3
1	D	159	HIS	3.3
1	B	140	LYS	3.2
1	D	160	GLN	3.0
1	B	152	VAL	2.9
1	A	41	HIS	2.9
1	B	40	GLY	2.8
1	B	39	ILE	2.8
1	B	2	SER	2.7
1	C	44	ASN	2.5
1	B	161	GLN	2.5
1	C	163	TRP	2.4
1	D	161	GLN	2.4
1	B	44	ASN	2.3
1	F	163	TRP	2.3
1	A	42	HIS	2.3
1	F	-5	VAL	2.2
1	E	162	GLY	2.2
1	F	-6	LEU	2.2
1	D	149	GLN	2.1
1	E	-6	LEU	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	CIT	B	201	13/13	0.81	0.14	2.08	46,57,62,68	0
2	CIT	D	201	13/13	0.89	0.12	0.90	40,48,56,58	0
2	CIT	C	201	13/13	0.92	0.10	0.81	38,42,44,45	0
2	CIT	F	201	13/13	0.94	0.08	0.04	33,41,46,54	0
2	CIT	A	201	13/13	0.92	0.09	-0.24	35,43,49,52	0
2	CIT	E	201	13/13	0.93	0.08	-0.35	39,43,54,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.