Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:17 PM GMT

PDB ID	:	1O9R
Title	:	THE X-RAY CRYSTAL STRUCTURE OF AGROBACTERIUM TUMEFACIENS DPS, A MEMBER OF THE FAMILY THAT PROTECT DNA WITHOUT BINDING
Authors	:	Ilari, A.; Ceci, P.; Chiancone, E.
Deposited on	:	2002-12-18
Resolution	:	1.45 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

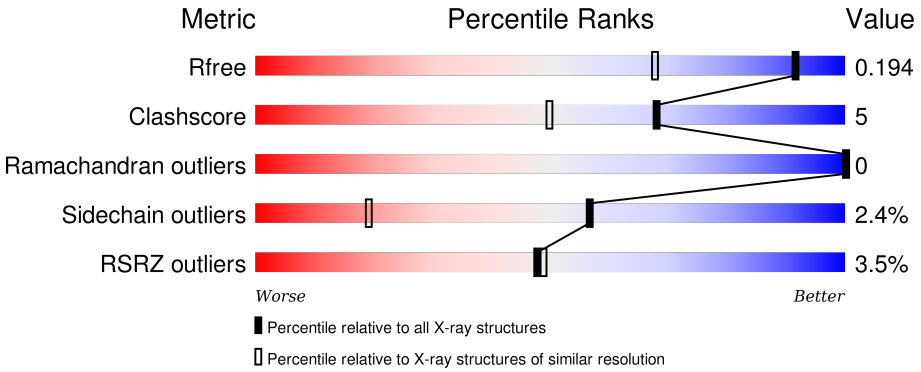
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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	162	3% 88% 9%
1	B	162	4% 85% 13%
1	C	162	3% 83% 13%
1	D	162	4% 84% 10%
1	E	162	3% 85% 13%

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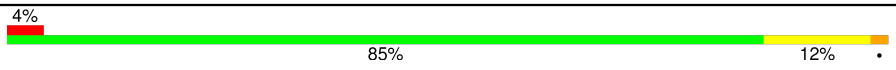
Mol	Chain	Length	Quality of chain
1	F	162	

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	FE	B	1163	-	-	-	X
2	FE	D	1163	-	-	-	X
3	TRS	B	1164	-	-	-	X
4	EDO	D	1164	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8286 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.

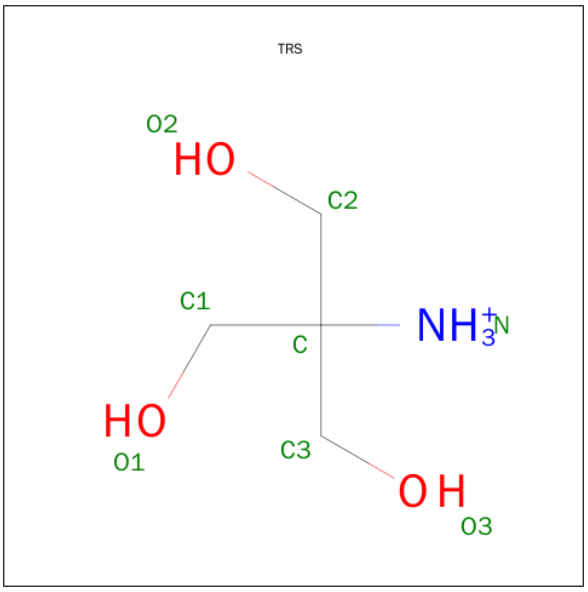
- Molecule 1 is a protein called AGROBACTERIUM TUMEFACIENS DPS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			
1	B	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			
1	C	159	Total	C	N	O	S	0	1	0
			1236	775	213	247	1			
1	D	160	Total	C	N	O	S	0	1	0
			1243	779	214	249	1			
1	E	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			
1	F	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

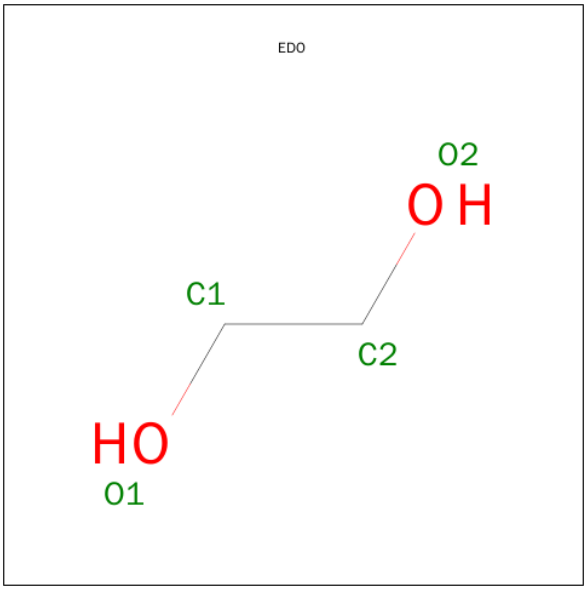
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 8 4 1 3	0	0
3	E	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

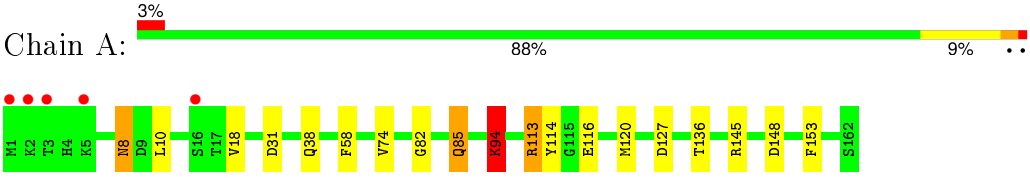
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	129	Total O 129 129	0	0
5	B	134	Total O 134 134	0	0
5	C	121	Total O 121 121	0	0
5	D	115	Total O 115 115	0	0
5	E	116	Total O 116 116	0	0
5	F	126	Total O 126 126	0	0

3 Residue-property plots (i)

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

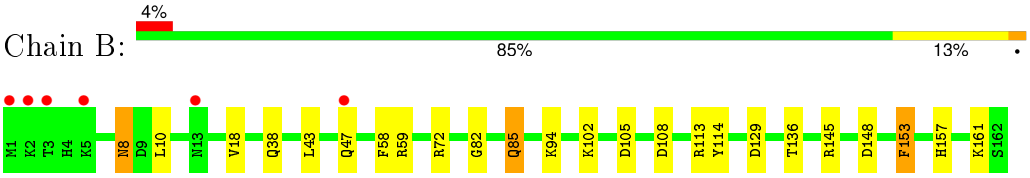
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS

Chain A:



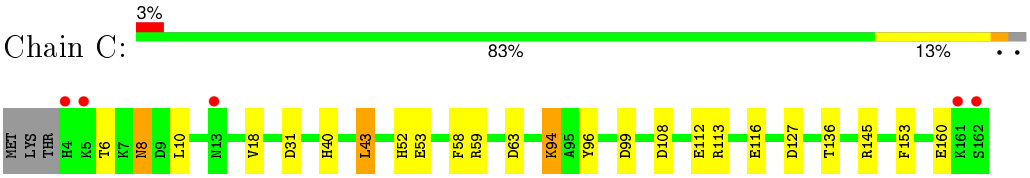
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS

Chain B:



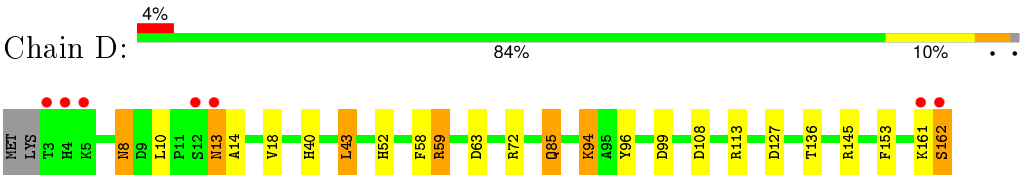
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS

Chain C:



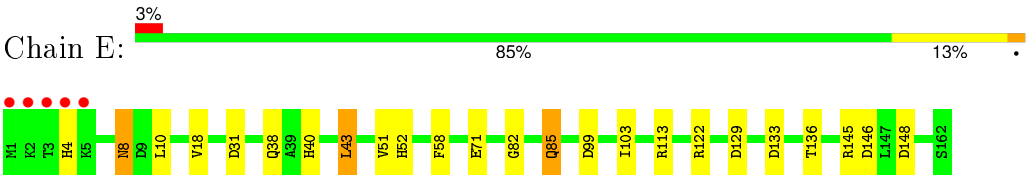
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS

Chain D:



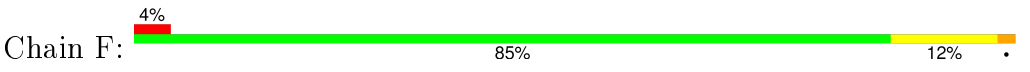
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS

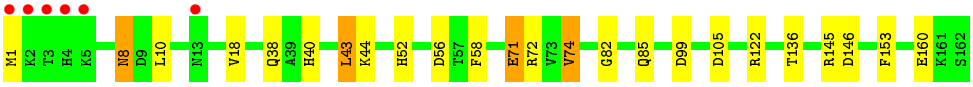
Chain E:



- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS

Chain F:




M1
K2
T3
H4
K5
N8
D9
L10
N13
V18
Q38
A39
H40
L43
K44
H52
D56
T57
F58
E71
R72
V73
V74
G82
Q85
D99
D105
R122
T136
R145
D146
F153
E160
K161
S162

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.05Å 90.35Å 105.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.45 32.92 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-1.45) 96.4 (32.92-1.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.200 0.170 , 0.194	Depositor DCC
R_{free} test set	8601 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 48.1	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 171823 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.30 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5536e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, FE, EDO

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	0/1285	1.48	16/1742 (0.9%)
1	B	0.86	0/1285	1.61	20/1742 (1.1%)
1	C	0.85	1/1261 (0.1%)	1.51	15/1711 (0.9%)
1	D	0.89	0/1268	1.52	16/1721 (0.9%)
1	E	0.86	0/1285	1.48	16/1742 (0.9%)
1	F	0.85	0/1285	1.43	14/1742 (0.8%)
All	All	0.86	1/7669 (0.0%)	1.50	97/10400 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	GLU	CD-OE1	-6.40	1.18	1.25

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	ARG	NE-CZ-NH1	16.81	128.71	120.30
1	E	145	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	B	161	LYS	CD-CE-NZ	13.43	142.59	111.70
1	E	43	LEU	CA-CB-CG	13.11	145.44	115.30
1	B	113	ARG	NE-CZ-NH2	-12.97	113.81	120.30
1	C	145	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	B	72	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	E	145	ARG	NE-CZ-NH2	-12.11	114.24	120.30
1	A	145	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	D	145	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	E	58	PHE	CB-CG-CD1	-10.94	113.14	120.80
1	F	145	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	C	113	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	C	99	ASP	CB-CG-OD2	10.67	127.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	D	127	ASP	CB-CG-OD1	-10.17	109.15	118.30
1	C	145	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	C	58	PHE	CB-CG-CD1	-10.09	113.74	120.80
1	D	99	ASP	CB-CG-OD2	9.63	126.97	118.30
1	B	72	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	113	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	B	59	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	A	58	PHE	CB-CG-CD1	-9.09	114.44	120.80
1	C	153	PHE	CB-CG-CD2	9.06	127.14	120.80
1	F	146	ASP	CB-CG-OD2	8.88	126.30	118.30
1	F	145	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	F	99	ASP	CB-CG-OD1	8.63	126.06	118.30
1	D	145	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	59	ARG	NE-CZ-NH1	-8.53	116.03	120.30
1	B	129	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	C	31	ASP	CB-CG-OD1	8.17	125.65	118.30
1	E	58	PHE	CB-CG-CD2	7.85	126.29	120.80
1	E	113	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	D	59	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	A	153	PHE	CB-CG-CD2	7.55	126.09	120.80
1	B	153	PHE	CB-CG-CD2	7.50	126.05	120.80
1	F	58	PHE	CB-CG-CD1	-7.44	115.59	120.80
1	D	63	ASP	CB-CG-OD1	-7.35	111.69	118.30
1	C	59	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	B	108	ASP	CB-CG-OD2	7.25	124.82	118.30
1	B	153	PHE	CB-CG-CD1	-7.21	115.75	120.80
1	B	114	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	B	145	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	D	58	PHE	CB-CG-CD1	-6.66	116.14	120.80
1	B	105	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	C	153	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	A	74	VAL	CA-CB-CG2	6.61	120.81	110.90
1	E	43	LEU	CB-CA-C	-6.50	97.86	110.20
1	E	145	ARG	CD-NE-CZ	-6.50	114.51	123.60
1	E	71	GLU	OE1-CD-OE2	-6.49	115.52	123.30
1	D	59	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	D	108	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	F	71	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	C	108	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	F	153	PHE	CB-CG-CD2	6.38	125.27	120.80
1	C	96	TYR	CB-CG-CD1	-6.22	117.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	122	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	D	113	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	127	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	113	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	114	TYR	CG-CD1-CE1	-6.11	116.41	121.30
1	F	74	VAL	CA-CB-CG2	6.07	120.00	110.90
1	F	105	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	A	94	LYS	CA-CB-CG	6.02	126.65	113.40
1	E	31	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	148	ASP	CB-CG-OD2	5.96	123.66	118.30
1	F	160	GLU	OE1-CD-OE2	5.93	130.42	123.30
1	D	108	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	148	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	B	58	PHE	CB-CG-CD1	-5.78	116.75	120.80
1	A	148	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	31	ASP	CB-CG-OD1	5.69	123.42	118.30
1	F	72	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	161	LYS	C-N-CA	-5.61	107.67	121.70
1	D	96	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	D	72	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	43	LEU	CB-CA-C	-5.51	99.72	110.20
1	E	129	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	F	153	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	C	6	THR	N-CA-CB	5.43	120.61	110.30
1	C	63	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	A	148	ASP	CB-CG-OD1	-5.32	113.52	118.30
1	C	127	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	D	162	SER	CB-CA-C	5.26	120.10	110.10
1	E	133	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	E	122	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	E	148	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	114	TYR	CG-CD1-CE1	-5.21	117.14	121.30
1	A	74	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	120	MET	CA-CB-CG	5.17	122.09	113.30
1	E	99	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	94	LYS	CB-CG-CD	5.14	124.97	111.60
1	A	114	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	145	ARG	CD-NE-CZ	-5.11	116.44	123.60
1	F	56	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	E	146	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	153	PHE	CB-CG-CD2	5.03	124.32	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1260	0	1255	19	0
1	B	1260	0	1255	13	0
1	C	1236	0	1223	12	0
1	D	1243	0	1230	11	0
1	E	1260	0	1255	14	0
1	F	1260	0	1255	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	8	0	12	0	0
3	E	8	0	12	0	0
4	D	4	0	5	0	0
5	A	129	0	0	0	0
5	B	134	0	0	0	0
5	C	121	0	0	0	1
5	D	115	0	0	1	0
5	E	116	0	0	0	0
5	F	126	0	0	0	0
All	All	8286	0	7502	71	1

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 (71) 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:94:LYS:NZ	1:A:113:ARG:HG2	1.88	0.89
1:A:94:LYS:HE3	1:A:94:LYS:H	1.39	0.84
1:A:94:LYS:HZ3	1:A:113:ARG:HG2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:HE22	1:B:82:GLY:H	1.31	0.78
1:C:94:LYS:HZ3	1:C:94:LYS:H	1.32	0.78
1:E:82:GLY:H	1:F:38:GLN:HE22	1.34	0.76
1:A:94:LYS:H	1:A:94:LYS:CE	1.99	0.75
1:A:38:GLN:NE2	1:B:82:GLY:H	1.86	0.74
1:A:82:GLY:H	1:B:38:GLN:HE22	1.34	0.73
1:E:38:GLN:HE22	1:F:82:GLY:H	1.37	0.71
1:A:82:GLY:H	1:B:38:GLN:NE2	1.91	0.69
1:E:82:GLY:H	1:F:38:GLN:NE2	1.92	0.67
1:E:38:GLN:NE2	1:F:82:GLY:H	1.94	0.64
1:D:94:LYS:HA	1:D:94:LYS:HE3	1.80	0.63
1:A:94:LYS:NZ	1:A:116:GLU:OE2	2.32	0.63
1:D:43:LEU:HD12	1:D:43:LEU:H	1.67	0.59
1:A:94:LYS:HZ3	1:A:113:ARG:CG	2.16	0.58
1:A:94:LYS:HZ2	1:A:113:ARG:HG2	1.65	0.57
1:C:94:LYS:N	1:C:94:LYS:HD3	2.19	0.56
1:C:94:LYS:NZ	1:C:94:LYS:H	2.04	0.55
1:D:59:ARG:NH1	5:D:2039:HOH:O	2.39	0.54
1:B:18:VAL:CG1	1:B:136:THR:HG21	2.38	0.53
1:C:8:ASN:HD22	1:C:8:ASN:C	2.14	0.51
1:F:8:ASN:HD22	1:F:10:LEU:H	1.58	0.50
1:B:153:PHE:O	1:B:157:HIS:HD2	1.93	0.50
1:D:40:HIS:O	1:D:52:HIS:HD2	1.95	0.50
1:B:8:ASN:HD22	1:B:10:LEU:H	1.58	0.49
1:D:18:VAL:CG1	1:D:136:THR:HG21	2.42	0.49
1:E:43:LEU:HD11	1:E:51:VAL:HG12	1.95	0.49
1:B:102:LYS:NZ	1:C:160:GLU:OE1	2.38	0.49
1:A:8:ASN:C	1:A:8:ASN:HD22	2.16	0.48
1:D:8:ASN:C	1:D:8:ASN:HD22	2.18	0.47
1:C:18:VAL:CG1	1:C:136:THR:HG21	2.45	0.47
1:B:18:VAL:HG13	1:B:136:THR:HG21	1.97	0.46
1:B:47:GLN:HG2	1:B:47:GLN:O	2.16	0.46
1:E:8:ASN:HD22	1:E:10:LEU:H	1.62	0.46
1:E:4:HIS:CE1	1:F:44:LYS:HE3	2.50	0.46
1:F:71:GLU:O	1:F:74:VAL:HG22	2.16	0.46
1:E:43:LEU:HD11	1:E:51:VAL:CG1	2.46	0.45
1:D:8:ASN:HD22	1:D:10:LEU:H	1.64	0.45
1:A:94:LYS:H	1:A:94:LYS:CD	2.29	0.44
1:C:94:LYS:CD	1:C:94:LYS:N	2.81	0.43
1:F:8:ASN:ND2	1:F:10:LEU:H	2.16	0.43
1:B:8:ASN:ND2	1:B:10:LEU:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:VAL:CG1	1:E:136:THR:HG21	2.48	0.43
1:D:13:ASN:HD22	1:D:14:ALA:H	1.64	0.43
1:C:94:LYS:HE2	1:C:112:GLU:OE1	2.18	0.43
1:E:8:ASN:HD22	1:E:8:ASN:C	2.22	0.43
1:A:94:LYS:CE	1:A:116:GLU:OE2	2.67	0.43
1:F:18:VAL:CG1	1:F:136:THR:HG21	2.49	0.43
1:A:18:VAL:CG1	1:A:136:THR:HG21	2.49	0.43
1:C:94:LYS:NZ	1:C:116:GLU:OE2	2.48	0.43
1:A:85:GLN:NE2	1:A:85:GLN:H	2.16	0.43
1:B:85:GLN:NE2	1:B:85:GLN:H	2.16	0.43
1:A:94:LYS:HD2	1:A:113:ARG:CZ	2.49	0.42
1:E:43:LEU:HD13	1:E:103:ILE:HG12	2.01	0.42
1:A:8:ASN:HD22	1:A:10:LEU:H	1.67	0.42
1:C:43:LEU:H	1:C:43:LEU:HD12	1.83	0.42
1:D:85:GLN:NE2	1:D:85:GLN:H	2.17	0.42
1:C:40:HIS:CE1	1:C:52:HIS:CE1	3.07	0.42
1:B:8:ASN:C	1:B:8:ASN:HD22	2.23	0.42
1:D:8:ASN:ND2	1:D:10:LEU:H	2.18	0.41
1:A:18:VAL:HG13	1:A:136:THR:HG21	2.01	0.41
1:E:40:HIS:CE1	1:E:52:HIS:CE1	3.08	0.41
1:E:8:ASN:ND2	1:E:10:LEU:H	2.18	0.41
1:D:43:LEU:HD12	1:D:43:LEU:N	2.34	0.41
1:F:85:GLN:H	1:F:85:GLN:NE2	2.18	0.41
1:F:40:HIS:CE1	1:F:52:HIS:CE1	3.09	0.41
1:C:8:ASN:HD22	1:C:10:LEU:H	1.69	0.41
1:F:43:LEU:HD12	1:F:43:LEU:H	1.86	0.41
1:E:85:GLN:H	1:E:85:GLN:NE2	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2046:HOH:O	5:C:2046:HOH:O[2_665]	1.34	0.86

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	161/162 (99%)	158 (98%)	3 (2%)	0	100	100
1	B	161/162 (99%)	160 (99%)	1 (1%)	0	100	100
1	C	158/162 (98%)	156 (99%)	2 (1%)	0	100	100
1	D	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
1	E	161/162 (99%)	160 (99%)	1 (1%)	0	100	100
1	F	161/162 (99%)	160 (99%)	1 (1%)	0	100	100
All	All	961/972 (99%)	951 (99%)	10 (1%)	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	138/137 (101%)	135 (98%)	3 (2%)	60	22
1	B	138/137 (101%)	135 (98%)	3 (2%)	60	22
1	C	135/137 (98%)	132 (98%)	3 (2%)	60	22
1	D	136/137 (99%)	130 (96%)	6 (4%)	35	5
1	E	138/137 (101%)	136 (99%)	2 (1%)	74	42
1	F	138/137 (101%)	135 (98%)	3 (2%)	60	22
All	All	823/822 (100%)	803 (98%)	20 (2%)	57	19

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	85	GLN
1	A	94	LYS

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Mol	Chain	Res	Type
1	B	8	ASN
1	B	85	GLN
1	B	94	LYS
1	C	8	ASN
1	C	43	LEU
1	C	94	LYS
1	D	8	ASN
1	D	13	ASN
1	D	43	LEU
1	D	85	GLN
1	D	94	LYS
1	D	162	SER
1	E	8	ASN
1	E	85	GLN
1	F	1	MET
1	F	8	ASN
1	F	43	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	GLN
1	A	85	GLN
1	B	8	ASN
1	B	38	GLN
1	B	47	GLN
1	B	85	GLN
1	B	104	HIS
1	B	157	HIS
1	C	8	ASN
1	C	38	GLN
1	C	85	GLN
1	D	8	ASN
1	D	13	ASN
1	D	52	HIS
1	D	85	GLN
1	E	8	ASN
1	E	38	GLN
1	E	85	GLN
1	E	104	HIS
1	F	8	ASN

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Mol	Chain	Res	Type
1	F	38	GLN
1	F	85	GLN

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

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TRS	B	1164	-	7,7,7	1.47	1 (14%)	9,9,9	0.97	0
4	EDO	D	1164	-	3,3,3	2.43	1 (33%)	2,2,2	0.91	0
3	TRS	E	1164	-	7,7,7	1.71	1 (14%)	9,9,9	1.39	2 (22%)

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
3	TRS	B	1164	-	-	0/9/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	1164	-	-	0/1/1/1	0/0/0/0
3	TRS	E	1164	-	-	0/9/9/9	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1164	TRS	C3-C	-4.23	1.44	1.53
3	B	1164	TRS	C3-C	-3.71	1.45	1.53
4	D	1164	EDO	O1-C1	3.61	1.61	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1164	TRS	O2-C2-C	2.43	116.09	111.18
3	E	1164	TRS	C3-C-N	2.56	112.74	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	162/162 (100%)	0.04	5 (3%)	52	53	13, 16, 25, 44	0
1	B	162/162 (100%)	0.03	6 (3%)	45	46	13, 16, 25, 43	0
1	C	159/162 (98%)	0.03	5 (3%)	52	53	13, 16, 24, 39	0
1	D	160/162 (98%)	0.06	7 (4%)	38	38	13, 16, 25, 50	0
1	E	162/162 (100%)	0.06	5 (3%)	52	53	13, 16, 25, 49	0
1	F	162/162 (100%)	0.06	6 (3%)	45	46	13, 16, 24, 49	0
All	All	967/972 (99%)	0.05	34 (3%)	48	49	13, 16, 25, 50	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	THR	8.2
1	F	3	THR	7.0
1	B	3	THR	6.7
1	E	3	THR	6.5
1	F	1	MET	6.3
1	A	1	MET	6.0
1	E	1	MET	5.9
1	A	3	THR	5.1
1	B	1	MET	4.5
1	D	4	HIS	4.5
1	D	161	LYS	4.1
1	D	162	SER	4.0
1	C	162	SER	3.8
1	E	2	LYS	3.8
1	D	5	LYS	3.8
1	F	2	LYS	3.7
1	F	4	HIS	3.6
1	C	13	ASN	3.3
1	C	5	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	5	LYS	3.2
1	E	5	LYS	3.2
1	A	2	LYS	3.1
1	C	161	LYS	3.1
1	B	2	LYS	3.0
1	F	5	LYS	2.6
1	B	47	GLN	2.5
1	C	4	HIS	2.5
1	B	5	LYS	2.5
1	E	4	HIS	2.4
1	D	13	ASN	2.3
1	F	13	ASN	2.2
1	D	12	SER	2.1
1	A	16	SER	2.1
1	B	13	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	FE	B	1163	1/1	0.92	0.21	4.55	27,27,27,27	1
2	FE	D	1163	1/1	0.94	0.15	3.71	29,29,29,29	1
4	EDO	D	1164	4/4	0.88	0.14	2.64	21,22,22,24	0
3	TRS	B	1164	8/8	0.95	0.10	2.05	14,15,16,16	0
2	FE	A	1163	1/1	0.92	0.16	1.53	25,25,25,25	1
2	FE	C	1163	1/1	0.86	0.12	1.46	31,31,31,31	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE	F	1163	1/1	0.94	0.12	1.41	28,28,28,28	1
2	FE	E	1163	1/1	0.95	0.12	1.35	27,27,27,27	1
3	TRS	E	1164	8/8	0.97	0.08	1.27	14,15,15,16	0

6.5 Other polymers (i)

There are no such residues in this entry.