Full wwPDB X-ray Structure Validation Report

Jun 17, 2024 – 02:46 AM EDT

PDB ID	:	5MUX
Title	:	Crystal structure of 2-methylcitrate dehydratase (MmgE) from Bacillus subtilis.
Authors	:	Baker, G.E.; Race, P.R.
Deposited on	:	2017-01-14
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

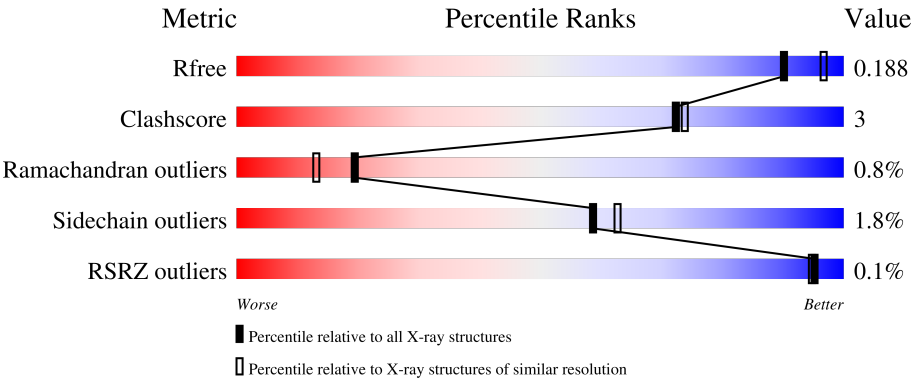
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	472	90% 7% •••
1	B	472	92% 7% ••
1	C	472	93% 6% •
1	D	472	93% 7% •
1	E	472	93% 5% •

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Mol	Chain	Length	Quality of chain
1	F	472	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23106 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.

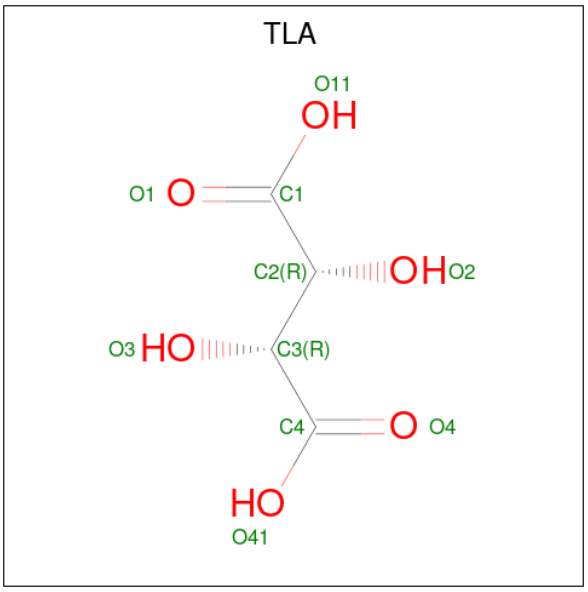
- Molecule 1 is a protein called 2-methylcitrate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3679	2325	645	693	16			
1	B	472	Total	C	N	O	S	0	0	0
			3683	2328	645	693	17			
1	C	472	Total	C	N	O	S	0	0	0
			3691	2335	647	692	17			
1	D	471	Total	C	N	O	S	0	0	0
			3686	2331	645	693	17			
1	E	472	Total	C	N	O	S	0	0	0
			3670	2325	641	687	17			
1	F	468	Total	C	N	O	S	0	0	0
			3611	2281	634	682	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	PRO	ALA	conflict	UNP P45859
B	216	PRO	ALA	conflict	UNP P45859
C	216	PRO	ALA	conflict	UNP P45859
D	216	PRO	ALA	conflict	UNP P45859
E	216	PRO	ALA	conflict	UNP P45859
F	216	PRO	ALA	conflict	UNP P45859

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	E	1	Total C O 10 4 6	0	0
2	F	1	Total C O 10 4 6	0	0

- Molecule 3 is water.

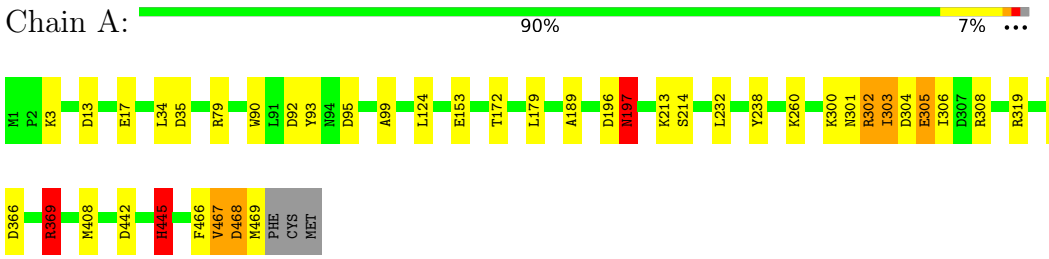
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	161	Total O 161 161	0	0
3	B	181	Total O 181 181	0	0
3	C	205	Total O 205 205	0	0
3	D	160	Total O 160 160	0	0
3	E	166	Total O 166 166	0	0
3	F	153	Total O 153 153	0	0

3 Residue-property plots (i)

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

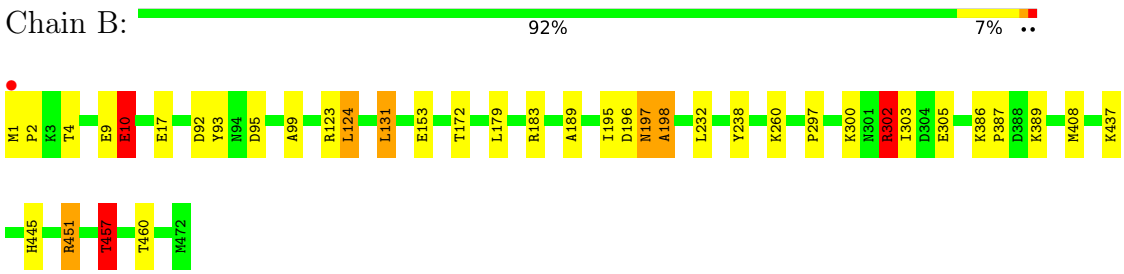
• Molecule 1: 2-methylcitrate dehydratase

Chain A:



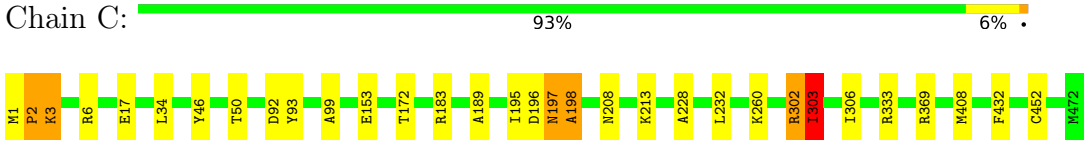
• Molecule 1: 2-methylcitrate dehydratase

Chain B:



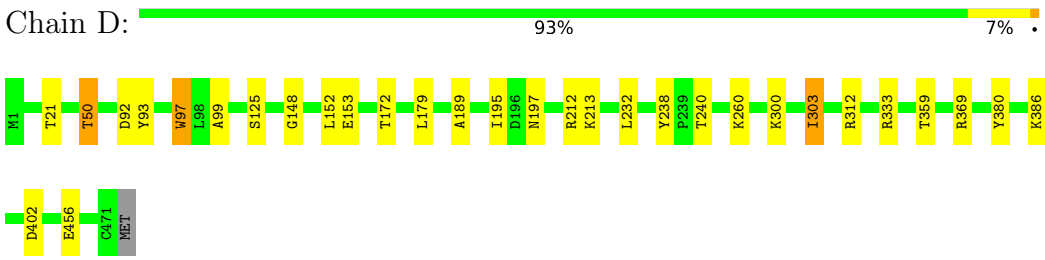
• Molecule 1: 2-methylcitrate dehydratase

Chain C:



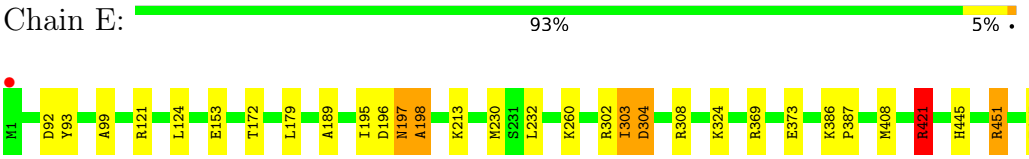
• Molecule 1: 2-methylcitrate dehydratase

Chain D:



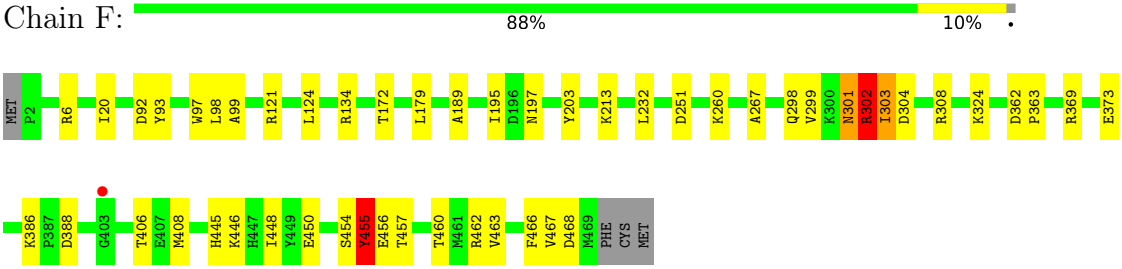
• Molecule 1: 2-methylcitrate dehydratase

Chain E:



• Molecule 1: 2-methylcitrate dehydratase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.83Å 194.41Å 90.87Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	30.80 – 2.00 30.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.80-2.00) 99.4 (30.80-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.151 , 0.189 0.152 , 0.188	Depositor DCC
R_{free} test set	10311 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 18.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.063 for l,k,-h 0.064 for h,-k,-l 0.448 for l,-k,h	Xtriage
Reported twinning fraction	0.525 for H, K, L 0.475 for L, -K, H	Depositor
Outliers	0 of 210387 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23106	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.67	1/3758 (0.0%)	0.80	5/5102 (0.1%)
1	B	0.75	4/3763 (0.1%)	0.81	4/5112 (0.1%)
1	C	0.71	0/3771	0.77	5/5120 (0.1%)
1	D	0.75	1/3766 (0.0%)	0.79	5/5112 (0.1%)
1	E	0.65	0/3750	0.77	5/5093 (0.1%)
1	F	0.68	1/3688 (0.0%)	0.79	6/5014 (0.1%)
All	All	0.70	7/22496 (0.0%)	0.79	30/30553 (0.1%)

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	A	0	7
1	B	0	3
1	C	0	4
1	D	0	1
1	E	0	3
1	F	2	3
All	All	2	21

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	GLU	CD-OE1	7.83	1.34	1.25
1	B	10	GLU	CG-CD	7.72	1.63	1.51
1	D	97	TRP	CB-CG	-6.37	1.38	1.50
1	B	10	GLU	CB-CG	5.65	1.62	1.52
1	B	10	GLU	CD-OE2	5.31	1.31	1.25
1	F	203	TYR	CE1-CZ	-5.22	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	ARG	CD-NE	-5.19	1.37	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	306	ILE	N-CA-C	-8.81	87.22	111.00
1	F	468	ASP	CB-CG-OD1	-7.89	111.19	118.30
1	B	302	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	E	230	MET	CG-SD-CE	-7.67	87.93	100.20
1	F	468	ASP	CB-CG-OD2	7.37	124.94	118.30
1	A	369	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	E	303	ILE	N-CA-C	-6.47	93.53	111.00
1	E	421	ARG	CG-CD-NE	-6.40	98.36	111.80
1	D	369	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	E	369	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	B	457	THR	N-CA-CB	6.25	122.19	110.30
1	D	369	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	333	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	369	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	212	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	F	97	TRP	N-CA-C	5.68	126.34	111.00
1	B	302	ARG	CD-NE-CZ	5.58	131.41	123.60
1	C	303	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	D	402	ASP	N-CA-CB	-5.48	100.74	110.60
1	F	251	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	319	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	451	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	369	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	445	HIS	CB-CA-C	5.09	120.58	110.40
1	F	260	LYS	CD-CE-NZ	5.08	123.39	111.70
1	D	333	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	333	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	451	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	369	ARG	NE-CZ-NH2	-5.02	117.79	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	307	ASP	CA
1	F	308	ARG	CA

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ASN	Peptide
1	A	238	TYR	Sidechain
1	A	302	ARG	Mainchain,Peptide
1	A	369	ARG	Sidechain
1	A	467	VAL	Mainchain
1	A	468	ASP	Peptide
1	B	196	ASP	Peptide
1	B	197	ASN	Peptide
1	B	238	TYR	Sidechain
1	C	196	ASP	Peptide
1	C	197	ASN	Peptide
1	C	2	PRO	Peptide
1	C	46	TYR	Sidechain
1	D	238	TYR	Sidechain
1	E	196	ASP	Peptide
1	E	197	ASN	Peptide
1	E	421	ARG	Sidechain
1	F	301	ASN	Peptide
1	F	302	ARG	Peptide
1	F	455	TYR	Peptide

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	3679	0	3648	22	0
1	B	3683	0	3625	32	0
1	C	3691	0	3649	24	0
1	D	3686	0	3644	22	1
1	E	3670	0	3619	18	0
1	F	3611	0	3520	36	1
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	161	0	0	1	0
3	B	181	0	0	2	0
3	C	205	0	0	0	0
3	D	160	0	0	1	0
3	E	166	0	0	1	0
3	F	153	0	0	3	0
All	All	23106	0	21729	147	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 3.

All (147) 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:F:460:THR:HG21	3:F:669:HOH:O	1.47	1.11
1:F:302:ARG:HA	1:F:303:ILE:HB	1.44	0.99
1:A:300:LYS:O	1:A:303:ILE:HG22	1.67	0.94
1:F:121:ARG:HH22	1:F:466:PHE:HE2	0.96	0.94
1:F:121:ARG:NH2	1:F:466:PHE:CE2	2.40	0.89
1:F:121:ARG:NH2	1:F:466:PHE:HE2	1.71	0.87
1:F:124:LEU:HD22	1:F:462:ARG:HD3	1.59	0.83
1:D:312:ARG:HG2	1:D:395:ALA:HB3	1.60	0.81
1:F:455:TYR:CG	1:F:456:GLU:N	2.46	0.81
1:F:455:TYR:CD2	1:F:456:GLU:N	2.50	0.79
1:F:302:ARG:HA	1:F:303:ILE:CB	2.14	0.77
1:B:300:LYS:O	1:B:303:ILE:HD11	1.89	0.73
1:C:2:PRO:HA	1:C:3:LYS:CB	2.18	0.72
1:D:97:TRP:CZ3	1:D:148:GLY:O	2.44	0.71
1:C:2:PRO:CA	1:C:3:LYS:CB	2.69	0.70
1:F:124:LEU:HD22	1:F:462:ARG:CD	2.22	0.69
1:D:456:GLU:N	1:D:456:GLU:OE1	2.26	0.68
1:A:466:PHE:O	1:A:468:ASP:N	2.24	0.68
1:B:437:LYS:HE2	1:B:445:HIS:CE1	2.29	0.67
1:E:197:ASN:CB	1:E:198:ALA:HB2	2.27	0.65
1:F:20:ILE:HD13	1:F:267:ALA:HB2	1.78	0.65
1:F:386:LYS:HE2	1:F:388:ASP:OD1	1.97	0.63
1:F:302:ARG:CA	1:F:303:ILE:HB	2.25	0.63
1:B:124:LEU:HD21	1:D:125:SER:O	1.99	0.62
1:B:4:THR:HG23	1:B:9:GLU:CG	2.30	0.62
1:E:308:ARG:NH1	1:E:373:GLU:OE2	2.29	0.62
1:F:446:LYS:O	1:F:450:GLU:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ASN:CB	1:B:198:ALA:HB2	2.30	0.61
1:E:302:ARG:C	1:E:303:ILE:O	2.35	0.61
1:C:197:ASN:CB	1:C:198:ALA:HB2	2.32	0.60
1:A:469:MET:HG2	3:A:734:HOH:O	2.02	0.59
1:C:302:ARG:O	1:C:303:ILE:HB	2.02	0.58
1:D:359:THR:N	3:D:601:HOH:O	2.36	0.58
1:F:301:ASN:O	1:F:302:ARG:CB	2.52	0.57
1:A:325:GLY:O	1:A:369:ARG:NH2	2.36	0.57
1:B:124:LEU:CD2	1:D:125:SER:O	2.52	0.57
1:D:303:ILE:H	1:D:303:ILE:HD13	1.70	0.57
1:E:303:ILE:O	1:E:304:ASP:CB	2.49	0.57
1:F:134:ARG:HB2	1:F:457:THR:HB	1.87	0.57
1:C:34:LEU:HD23	1:C:432:PHE:CD2	2.39	0.57
1:F:298:GLN:HG2	1:F:406:THR:HG22	1.86	0.56
1:B:302:ARG:HH11	1:B:302:ARG:HG2	1.71	0.56
1:D:386:LYS:HE3	1:D:388:ASP:OD1	2.06	0.55
1:F:448:ILE:HG12	1:F:467:VAL:HG12	1.88	0.55
1:B:303:ILE:HD12	1:B:303:ILE:H	1.71	0.54
1:B:1:MET:CB	1:B:2:PRO:CD	2.85	0.54
1:D:312:ARG:HG3	1:D:380:TYR:CE2	2.43	0.53
1:D:172:THR:CG2	1:D:189:ALA:HB1	2.38	0.52
1:B:197:ASN:CA	1:B:198:ALA:HB2	2.39	0.52
1:A:172:THR:CG2	1:A:189:ALA:HB1	2.40	0.52
1:B:172:THR:CG2	1:B:189:ALA:HB1	2.40	0.51
1:C:198:ALA:N	1:D:197:ASN:HB2	2.26	0.51
1:C:197:ASN:CA	1:C:198:ALA:HB2	2.41	0.51
1:C:198:ALA:H	1:D:197:ASN:HB2	1.76	0.51
1:E:197:ASN:CA	1:E:198:ALA:HB2	2.40	0.51
1:E:302:ARG:O	1:E:303:ILE:C	2.49	0.51
1:A:13:ASP:O	1:A:17:GLU:HG2	2.11	0.51
1:B:297:PRO:HA	1:B:300:LYS:HG2	1.93	0.51
1:E:172:THR:CG2	1:E:189:ALA:HB1	2.41	0.50
1:C:303:ILE:HA	1:C:306:ILE:HD12	1.93	0.50
1:C:172:THR:CG2	1:C:189:ALA:HB1	2.41	0.50
1:A:303:ILE:H	1:A:303:ILE:HD13	1.76	0.50
1:B:10:GLU:HG2	3:B:643:HOH:O	2.12	0.50
1:A:303:ILE:HG12	1:A:304:ASP:H	1.76	0.49
1:C:6:ARG:HB2	1:C:6:ARG:NH1	2.27	0.49
1:C:302:ARG:O	1:C:303:ILE:CB	2.61	0.49
1:D:50:THR:HG21	3:F:665:HOH:O	2.11	0.49
1:D:300:LYS:O	1:D:303:ILE:CD1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:HD23	1:C:432:PHE:CE2	2.48	0.49
1:D:312:ARG:HG3	1:D:380:TYR:HE2	1.77	0.48
1:B:131:LEU:N	1:B:131:LEU:CD1	2.76	0.48
1:F:172:THR:CG2	1:F:189:ALA:HB1	2.43	0.48
1:A:366:ASP:HA	1:A:369:ARG:HH11	1.79	0.48
1:B:437:LYS:HE2	1:B:445:HIS:HE1	1.75	0.48
1:A:303:ILE:HG12	1:A:304:ASP:N	2.29	0.48
1:C:208:ASN:HD21	1:D:240:THR:H	1.62	0.47
1:A:301:ASN:C	1:A:303:ILE:HG23	2.35	0.47
1:B:4:THR:HG23	1:B:9:GLU:HG3	1.95	0.47
1:F:302:ARG:HA	1:F:303:ILE:CG2	2.45	0.46
1:B:153:GLU:OE1	1:B:260:LYS:HE2	2.15	0.46
1:C:153:GLU:OE1	1:C:260:LYS:HE2	2.16	0.46
1:B:17:GLU:OE2	1:B:183:ARG:NH2	2.37	0.46
1:E:153:GLU:OE1	1:E:260:LYS:HE2	2.15	0.46
1:F:462:ARG:HG3	1:F:463:VAL:N	2.30	0.46
1:A:153:GLU:OE1	1:A:260:LYS:HE2	2.16	0.46
1:C:2:PRO:CB	1:C:3:LYS:CB	2.93	0.46
1:D:153:GLU:OE1	1:D:260:LYS:HE2	2.15	0.46
1:A:90:TRP:CE3	1:A:214:SER:HB3	2.52	0.45
1:C:34:LEU:HD21	1:C:452:CYS:HB3	1.98	0.45
1:D:179:LEU:HB3	1:D:232:LEU:HD21	1.99	0.45
1:B:451:ARG:HH12	1:B:457:THR:HG23	1.80	0.45
1:D:195:ILE:O	1:D:195:ILE:CG2	2.64	0.45
1:F:195:ILE:O	1:F:195:ILE:CG2	2.65	0.45
1:F:386:LYS:HG2	1:F:388:ASP:OD1	2.17	0.45
1:F:303:ILE:CG2	1:F:304:ASP:H	2.31	0.44
1:C:195:ILE:O	1:C:195:ILE:CG2	2.66	0.44
1:B:179:LEU:HB3	1:B:232:LEU:HD21	2.00	0.44
1:E:451:ARG:HH12	1:E:457:THR:HG23	1.83	0.44
1:B:386:LYS:HA	1:B:387:PRO:HD3	1.79	0.44
1:B:195:ILE:O	1:B:195:ILE:CG2	2.66	0.44
1:F:303:ILE:CG2	1:F:304:ASP:N	2.81	0.43
1:D:97:TRP:HH2	1:D:152:LEU:CD2	2.31	0.43
1:C:302:ARG:HH11	1:C:302:ARG:HG2	1.84	0.43
1:A:304:ASP:OD1	1:A:305:GLU:N	2.51	0.43
1:E:198:ALA:N	1:F:197:ASN:HB2	2.33	0.43
1:B:386:LYS:HE3	1:B:389:LYS:HB2	2.01	0.43
1:C:1:MET:HA	1:C:2:PRO:HD3	1.93	0.43
1:E:198:ALA:H	1:F:197:ASN:HB2	1.84	0.43
1:C:6:ARG:HB2	1:C:6:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:O	1:A:305:GLU:HG2	2.19	0.43
1:E:179:LEU:HB3	1:E:232:LEU:HD21	2.01	0.43
1:B:4:THR:CG2	1:B:9:GLU:CG	2.97	0.43
1:A:179:LEU:HB3	1:A:232:LEU:HD21	2.00	0.42
1:B:302:ARG:NH1	1:B:305:GLU:OE2	2.52	0.42
1:C:17:GLU:OE2	1:C:183:ARG:NH2	2.42	0.42
1:E:121:ARG:HD3	3:E:666:HOH:O	2.18	0.42
1:C:2:PRO:HB3	1:C:3:LYS:CB	2.50	0.42
1:B:451:ARG:NH1	1:B:457:THR:HG23	2.34	0.42
1:F:448:ILE:HG12	1:F:467:VAL:CG1	2.50	0.42
1:A:196:ASP:O	1:A:197:ASN:C	2.58	0.42
1:B:4:THR:HG23	1:B:9:GLU:CD	2.39	0.42
1:F:303:ILE:HG23	1:F:304:ASP:N	2.34	0.42
1:F:454:SER:O	1:F:456:GLU:HB3	2.20	0.41
1:B:195:ILE:C	1:B:197:ASN:H	2.24	0.41
1:D:386:LYS:HA	1:D:387:PRO:HD3	1.91	0.41
1:F:299:VAL:HG13	1:F:303:ILE:HD12	2.03	0.41
1:B:123:ARG:NH1	1:B:131:LEU:HD12	2.36	0.41
1:E:324:LYS:HE3	1:E:324:LYS:HB3	1.85	0.41
1:A:302:ARG:O	1:A:305:GLU:O	2.38	0.41
1:F:179:LEU:HB3	1:F:232:LEU:HD21	2.02	0.41
1:B:460:THR:HG23	3:B:659:HOH:O	2.20	0.41
1:E:179:LEU:HB3	1:E:232:LEU:CD2	2.51	0.41
1:E:386:LYS:HA	1:E:387:PRO:HD3	1.77	0.41
1:A:34:LEU:HD12	1:A:35:ASP:N	2.36	0.41
1:C:228:ALA:O	1:C:232:LEU:HD23	2.21	0.41
1:E:195:ILE:O	1:E:195:ILE:CG2	2.66	0.41
1:F:299:VAL:CG1	1:F:303:ILE:HD12	2.50	0.41
1:F:446:LYS:NZ	3:F:603:HOH:O	2.38	0.40
1:B:95:ASP:C	1:B:95:ASP:OD1	2.59	0.40
1:D:179:LEU:HB3	1:D:232:LEU:CD2	2.50	0.40
1:A:442:ASP:HA	1:A:445:HIS:ND1	2.37	0.40
1:A:468:ASP:C	1:A:469:MET:HG3	2.42	0.40
1:F:197:ASN:O	1:F:197:ASN:CG	2.60	0.40
1:A:95:ASP:OD1	1:A:95:ASP:C	2.60	0.40
1:B:131:LEU:N	1:B:131:LEU:HD12	2.37	0.40
1:E:195:ILE:C	1:E:197:ASN:H	2.25	0.40
1:F:362:ASP:HA	1:F:363:PRO:HD3	1.96	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)
1:D:21:THR:OG1	1:F:6:ARG:NH1[1_556]	2.17	0.03

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	467/472 (99%)	451 (97%)	11 (2%)	5 (1%)	14 8
1	B	470/472 (100%)	458 (97%)	9 (2%)	3 (1%)	25 19
1	C	470/472 (100%)	457 (97%)	9 (2%)	4 (1%)	17 11
1	D	469/472 (99%)	461 (98%)	7 (2%)	1 (0%)	47 44
1	E	470/472 (100%)	459 (98%)	8 (2%)	3 (1%)	25 19
1	F	466/472 (99%)	450 (97%)	10 (2%)	6 (1%)	12 6
All	All	2812/2832 (99%)	2736 (97%)	54 (2%)	22 (1%)	19 13

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ALA
1	C	198	ALA
1	C	303	ILE
1	E	198	ALA
1	F	302	ARG
1	F	303	ILE
1	F	308	ARG
1	A	305	GLU
1	B	457	THR
1	C	3	LYS
1	F	455	TYR
1	A	467	VAL
1	E	304	ASP
1	F	98	LEU
1	A	3	LYS

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Mol	Chain	Res	Type
1	C	99	ALA
1	D	99	ALA
1	F	99	ALA
1	A	99	ALA
1	B	99	ALA
1	E	99	ALA
1	A	197	ASN

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	394/402 (98%)	384 (98%)	10 (2%)	47	49
1	B	391/402 (97%)	384 (98%)	7 (2%)	59	63
1	C	393/402 (98%)	387 (98%)	6 (2%)	65	69
1	D	393/402 (98%)	388 (99%)	5 (1%)	69	74
1	E	388/402 (96%)	381 (98%)	7 (2%)	59	63
1	F	376/402 (94%)	368 (98%)	8 (2%)	53	57
All	All	2335/2412 (97%)	2292 (98%)	43 (2%)	59	63

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	92	ASP
1	A	93	TYR
1	A	124	LEU
1	A	213	LYS
1	A	303	ILE
1	A	308	ARG
1	A	334	ASP
1	A	408	MET
1	A	445	HIS
1	B	10	GLU

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Mol	Chain	Res	Type
1	B	92	ASP
1	B	93	TYR
1	B	124	LEU
1	B	131	LEU
1	B	302	ARG
1	B	408	MET
1	C	50	THR
1	C	92	ASP
1	C	93	TYR
1	C	213	LYS
1	C	302	ARG
1	C	408	MET
1	D	50	THR
1	D	92	ASP
1	D	93	TYR
1	D	213	LYS
1	D	303	ILE
1	E	92	ASP
1	E	93	TYR
1	E	124	LEU
1	E	213	LYS
1	E	408	MET
1	E	421	ARG
1	E	445	HIS
1	F	92	ASP
1	F	93	TYR
1	F	213	LYS
1	F	324	LYS
1	F	373	GLU
1	F	408	MET
1	F	445	HIS
1	F	455	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	208	ASN

5.3.3 RNA

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 monosaccharides 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	TLA	D	501	-	9,9,9	1.45	1 (11%)	12,12,12	1.50	2 (16%)
2	TLA	E	501	-	9,9,9	1.15	1 (11%)	12,12,12	1.61	4 (33%)
2	TLA	A	501	-	9,9,9	1.32	1 (11%)	12,12,12	1.39	2 (16%)
2	TLA	C	501	-	9,9,9	1.09	0	12,12,12	2.11	3 (25%)
2	TLA	B	501	-	9,9,9	1.65	2 (22%)	12,12,12	0.76	0
2	TLA	F	501	-	9,9,9	1.16	0	12,12,12	1.46	2 (16%)

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	TLA	D	501	-	-	3/12/12/12	-
2	TLA	E	501	-	-	4/12/12/12	-
2	TLA	A	501	-	-	3/12/12/12	-
2	TLA	C	501	-	-	2/12/12/12	-
2	TLA	B	501	-	-	2/12/12/12	-
2	TLA	F	501	-	-	3/12/12/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	TLA	C2-C1	-2.81	1.48	1.52
2	B	501	TLA	O1-C1	2.58	1.30	1.22
2	A	501	TLA	C3-C4	-2.13	1.49	1.52
2	D	501	TLA	O41-C4	-2.13	1.23	1.30
2	E	501	TLA	C2-C1	-2.08	1.49	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	TLA	O3-C3-C4	-4.49	101.25	110.66
2	C	501	TLA	O11-C1-C2	3.97	124.01	113.27
2	E	501	TLA	O11-C1-C2	2.99	121.36	113.27
2	E	501	TLA	O1-C1-C2	-2.78	114.31	121.63
2	F	501	TLA	O2-C2-C1	-2.66	105.08	110.66
2	A	501	TLA	O41-C4-C3	2.64	120.42	113.27
2	A	501	TLA	O4-C4-C3	-2.59	114.82	121.63
2	D	501	TLA	O41-C4-O4	-2.53	118.35	124.09
2	F	501	TLA	O11-C1-C2	2.45	119.88	113.27
2	E	501	TLA	O3-C3-C4	-2.36	105.73	110.66
2	C	501	TLA	O1-C1-C2	-2.07	116.18	121.63
2	D	501	TLA	O3-C3-C4	-2.05	106.37	110.66
2	E	501	TLA	O4-C4-C3	-2.02	116.31	121.63

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TLA	C1-C2-C3-C4
2	F	501	TLA	C1-C2-C3-C4
2	D	501	TLA	O2-C2-C3-O3
2	C	501	TLA	C1-C2-C3-C4
2	B	501	TLA	C1-C2-C3-C4
2	D	501	TLA	C1-C2-C3-C4
2	D	501	TLA	C2-C3-C4-O4
2	E	501	TLA	O1-C1-C2-C3
2	F	501	TLA	O1-C1-C2-C3
2	E	501	TLA	C1-C2-C3-C4
2	E	501	TLA	O11-C1-C2-C3
2	F	501	TLA	O2-C2-C3-O3
2	A	501	TLA	O2-C2-C3-O3
2	B	501	TLA	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	501	TLA	O2-C2-C3-O3
2	E	501	TLA	O2-C2-C3-O3
2	A	501	TLA	O11-C1-C2-C3

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	469/472 (99%)	-0.99	0 100 100	8, 18, 33, 56	0
1	B	472/472 (100%)	-0.99	1 (0%) 95 94	7, 16, 33, 65	0
1	C	472/472 (100%)	-0.95	0 100 100	6, 16, 37, 60	0
1	D	471/472 (99%)	-0.97	0 100 100	6, 16, 34, 62	0
1	E	472/472 (100%)	-0.96	1 (0%) 95 94	10, 20, 35, 74	0
1	F	468/472 (99%)	-0.83	1 (0%) 95 94	8, 20, 53, 75	0
All	All	2824/2832 (99%)	-0.95	3 (0%) 95 95	6, 18, 37, 75	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	403	GLY	2.7
1	B	1	MET	2.4
1	E	1	MET	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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. 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	B-factors(Å^2)	Q<0.9
2	TLA	B	501	10/10	0.98	0.08	12,18,21,23	0
2	TLA	C	501	10/10	0.98	0.07	15,17,18,21	0
2	TLA	F	501	10/10	0.98	0.08	17,22,30,31	0
2	TLA	D	501	10/10	0.99	0.05	10,13,15,18	0
2	TLA	E	501	10/10	0.99	0.07	22,25,28,29	0
2	TLA	A	501	10/10	0.99	0.06	17,23,28,30	0

6.5 Other polymers (i)

There are no such residues in this entry.