Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 05:19 pm GMT

PDB ID	:	6QGA
Title	:	Crystal structure of Ideonella sakaiensis MHETase bound to the non-hydrolyzable ligand MHETA
Authors	:	Palm, G.J.; Reisky, L.; Boettcher, D.; Mueller, H.; Michels, E.A.P.; Walczak, C.; Berndt, L.; Weiss, M.S.; Bornscheuer, U.T.; Weber, G.
Deposited on	:	2019-01-10
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

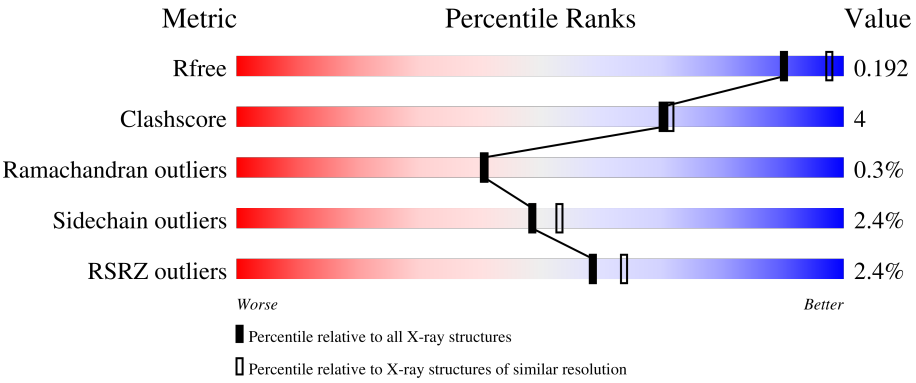
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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.



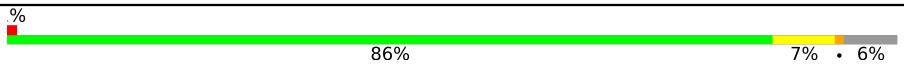
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	596	5% 85% 8% • 6%
1	B	596	2% 86% 7% • 6%
1	C	596	% 84% 9% • 7%
1	D	596	3% 86% 8% 6%
1	E	596	2% 87% 6% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	596	

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
6	CL	B	707	-	-	X	-
6	CL	C	704	-	-	X	-
6	CL	E	706	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27633 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 Mono(2-hydroxyethyl) terephthalate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4121	2581	724	788	28			
1	B	558	Total	C	N	O	S	0	1	0
			4136	2590	728	790	28			
1	C	557	Total	C	N	O	S	5	1	0
			4122	2584	723	786	29			
1	D	559	Total	C	N	O	S	0	0	0
			4129	2586	725	790	28			
1	E	558	Total	C	N	O	S	0	0	0
			4125	2584	724	789	28			
1	F	559	Total	C	N	O	S	0	1	0
			4134	2590	725	790	29			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP A0A0K8P8E7
A	9	ASN	-	expression tag	UNP A0A0K8P8E7
A	10	HIS	-	expression tag	UNP A0A0K8P8E7
A	11	LYS	-	expression tag	UNP A0A0K8P8E7
A	12	VAL	-	expression tag	UNP A0A0K8P8E7
A	13	HIS	-	expression tag	UNP A0A0K8P8E7
A	14	HIS	-	expression tag	UNP A0A0K8P8E7
A	15	HIS	-	expression tag	UNP A0A0K8P8E7
A	16	HIS	-	expression tag	UNP A0A0K8P8E7
A	17	HIS	-	expression tag	UNP A0A0K8P8E7
A	18	HIS	-	expression tag	UNP A0A0K8P8E7
A	19	MET	-	expression tag	UNP A0A0K8P8E7
B	8	MET	-	initiating methionine	UNP A0A0K8P8E7
B	9	ASN	-	expression tag	UNP A0A0K8P8E7
B	10	HIS	-	expression tag	UNP A0A0K8P8E7
B	11	LYS	-	expression tag	UNP A0A0K8P8E7
B	12	VAL	-	expression tag	UNP A0A0K8P8E7

Continued on next page...

Continued from previous page...

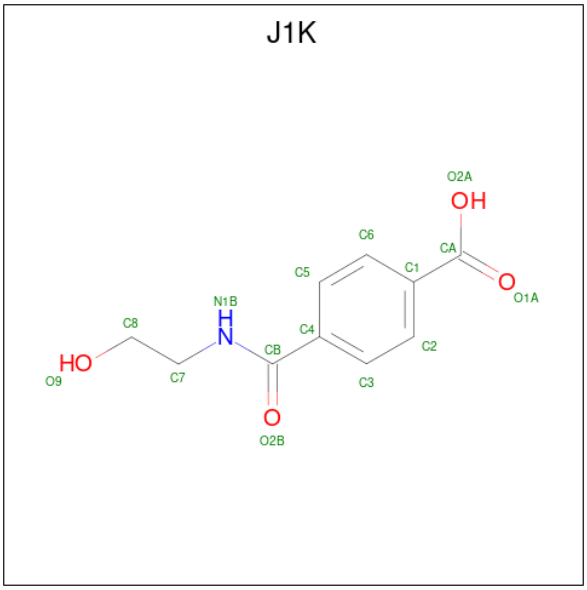
Chain	Residue	Modelled	Actual	Comment	Reference
B	13	HIS	-	expression tag	UNP A0A0K8P8E7
B	14	HIS	-	expression tag	UNP A0A0K8P8E7
B	15	HIS	-	expression tag	UNP A0A0K8P8E7
B	16	HIS	-	expression tag	UNP A0A0K8P8E7
B	17	HIS	-	expression tag	UNP A0A0K8P8E7
B	18	HIS	-	expression tag	UNP A0A0K8P8E7
B	19	MET	-	expression tag	UNP A0A0K8P8E7
C	8	MET	-	initiating methionine	UNP A0A0K8P8E7
C	9	ASN	-	expression tag	UNP A0A0K8P8E7
C	10	HIS	-	expression tag	UNP A0A0K8P8E7
C	11	LYS	-	expression tag	UNP A0A0K8P8E7
C	12	VAL	-	expression tag	UNP A0A0K8P8E7
C	13	HIS	-	expression tag	UNP A0A0K8P8E7
C	14	HIS	-	expression tag	UNP A0A0K8P8E7
C	15	HIS	-	expression tag	UNP A0A0K8P8E7
C	16	HIS	-	expression tag	UNP A0A0K8P8E7
C	17	HIS	-	expression tag	UNP A0A0K8P8E7
C	18	HIS	-	expression tag	UNP A0A0K8P8E7
C	19	MET	-	expression tag	UNP A0A0K8P8E7
D	8	MET	-	initiating methionine	UNP A0A0K8P8E7
D	9	ASN	-	expression tag	UNP A0A0K8P8E7
D	10	HIS	-	expression tag	UNP A0A0K8P8E7
D	11	LYS	-	expression tag	UNP A0A0K8P8E7
D	12	VAL	-	expression tag	UNP A0A0K8P8E7
D	13	HIS	-	expression tag	UNP A0A0K8P8E7
D	14	HIS	-	expression tag	UNP A0A0K8P8E7
D	15	HIS	-	expression tag	UNP A0A0K8P8E7
D	16	HIS	-	expression tag	UNP A0A0K8P8E7
D	17	HIS	-	expression tag	UNP A0A0K8P8E7
D	18	HIS	-	expression tag	UNP A0A0K8P8E7
D	19	MET	-	expression tag	UNP A0A0K8P8E7
E	8	MET	-	initiating methionine	UNP A0A0K8P8E7
E	9	ASN	-	expression tag	UNP A0A0K8P8E7
E	10	HIS	-	expression tag	UNP A0A0K8P8E7
E	11	LYS	-	expression tag	UNP A0A0K8P8E7
E	12	VAL	-	expression tag	UNP A0A0K8P8E7
E	13	HIS	-	expression tag	UNP A0A0K8P8E7
E	14	HIS	-	expression tag	UNP A0A0K8P8E7
E	15	HIS	-	expression tag	UNP A0A0K8P8E7
E	16	HIS	-	expression tag	UNP A0A0K8P8E7
E	17	HIS	-	expression tag	UNP A0A0K8P8E7
E	18	HIS	-	expression tag	UNP A0A0K8P8E7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	19	MET	-	expression tag	UNP A0A0K8P8E7
F	8	MET	-	initiating methionine	UNP A0A0K8P8E7
F	9	ASN	-	expression tag	UNP A0A0K8P8E7
F	10	HIS	-	expression tag	UNP A0A0K8P8E7
F	11	LYS	-	expression tag	UNP A0A0K8P8E7
F	12	VAL	-	expression tag	UNP A0A0K8P8E7
F	13	HIS	-	expression tag	UNP A0A0K8P8E7
F	14	HIS	-	expression tag	UNP A0A0K8P8E7
F	15	HIS	-	expression tag	UNP A0A0K8P8E7
F	16	HIS	-	expression tag	UNP A0A0K8P8E7
F	17	HIS	-	expression tag	UNP A0A0K8P8E7
F	18	HIS	-	expression tag	UNP A0A0K8P8E7
F	19	MET	-	expression tag	UNP A0A0K8P8E7

- Molecule 2 is 4-(2-hydroxyethylcarbamoyl)benzoic acid (three-letter code: J1K) (formula: $C_{10}H_{11}NO_4$).



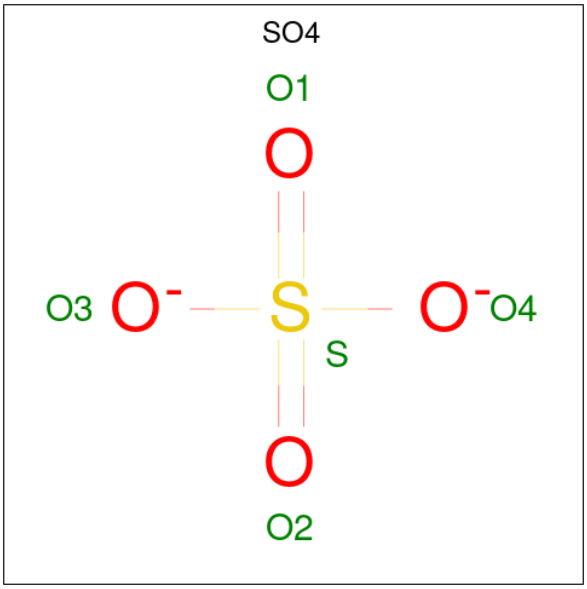
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 15 10 1 4	0	0
2	E	1	Total C N O 15 10 1 4	0	0
2	E	1	Total C N O 15 10 1 4	0	0
2	E	1	Total C N O 15 10 1 4	0	0
2	F	1	Total C N O 15 10 1 4	0	0
2	F	1	Total C N O 15 10 1 4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



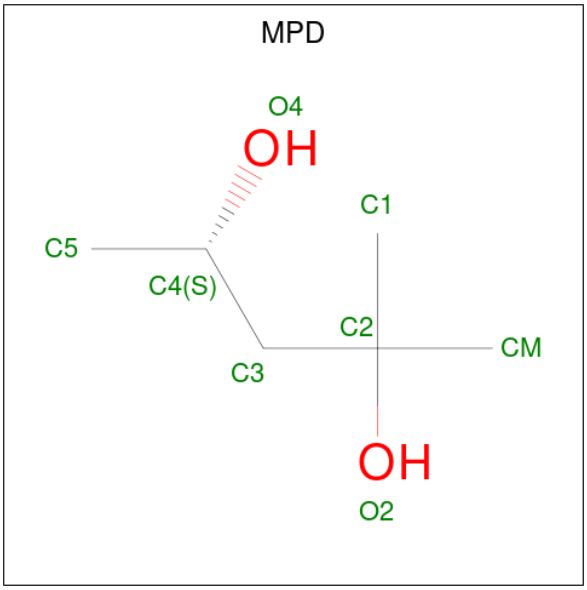
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	C	2	Total Cl 2 2	0	0
6	E	1	Total Cl 1 1	0	0

- Molecule 7 is water.

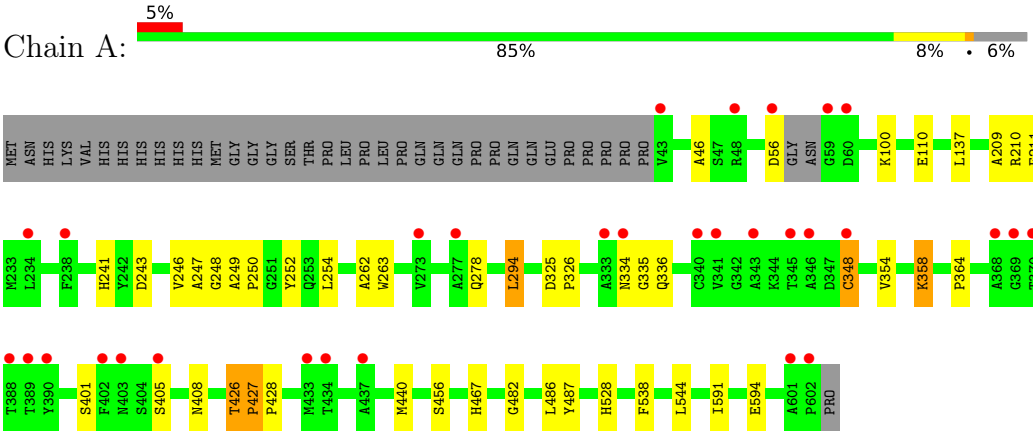
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	390	Total O 390 390	0	0
7	B	488	Total O 488 488	0	0
7	C	424	Total O 424 424	0	0
7	D	412	Total O 412 412	0	0
7	E	490	Total O 490 490	0	0
7	F	436	Total O 436 436	0	0

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.

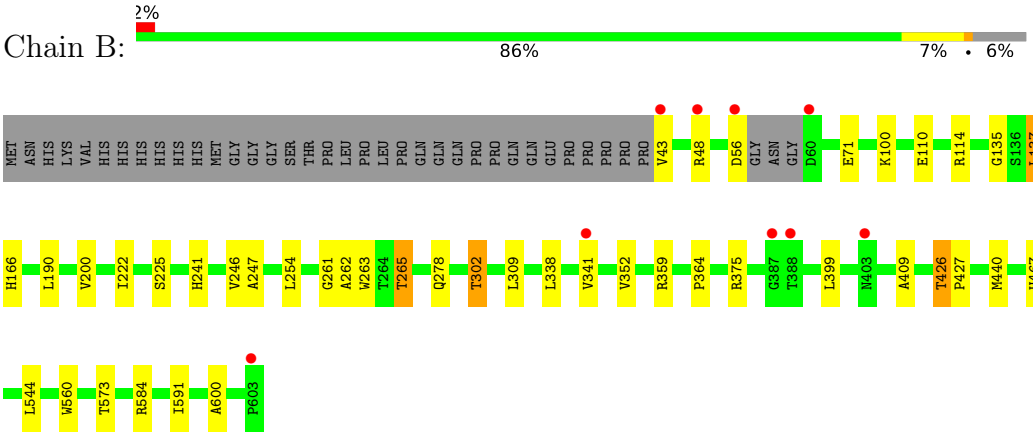
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain A:



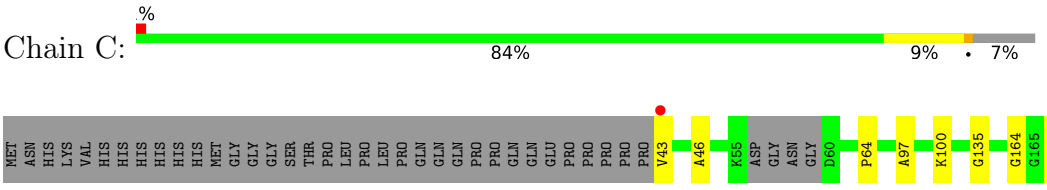
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

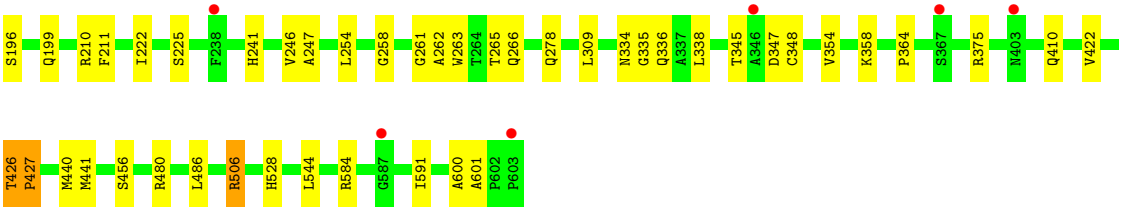
Chain B:



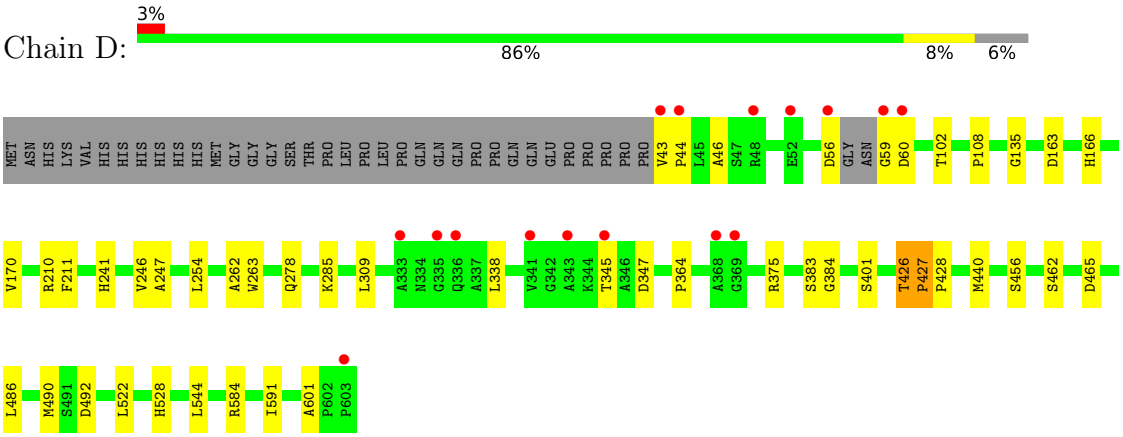
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase

Chain C:

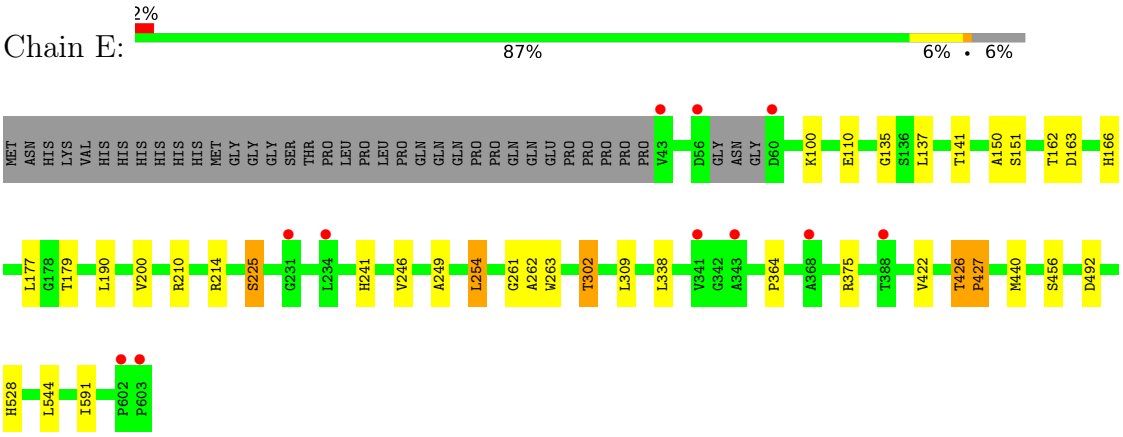




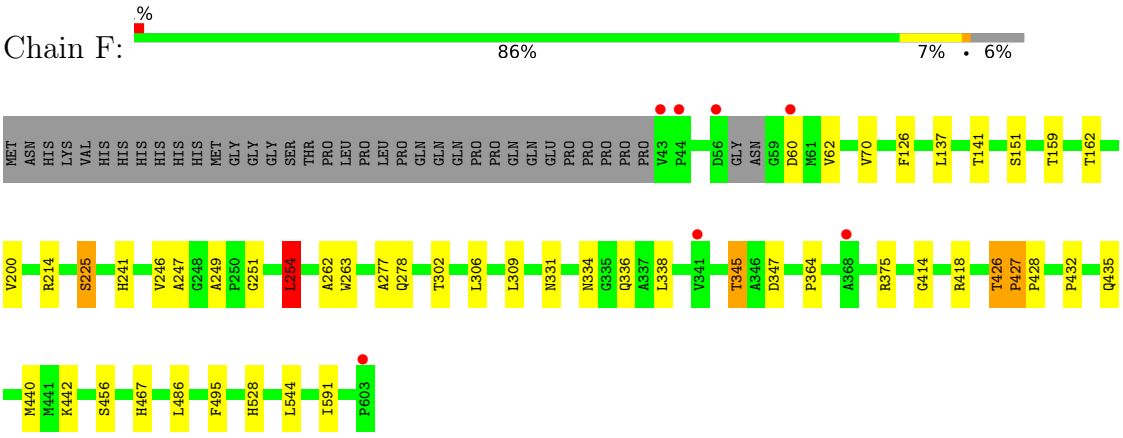
• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



• Molecule 1: Mono(2-hydroxyethyl) terephthalate hydrolase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.15Å 183.65Å 246.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 2.10 49.11 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.11-2.10) 98.9 (49.11-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.173 , 0.198 0.173 , 0.192	Depositor DCC
R_{free} test set	3081 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27633	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.98% 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: MPD, CL, CA, SO4, J1K

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	0.46	1/4227 (0.0%)	0.60	1/5754 (0.0%)
1	B	0.50	0/4243	0.66	3/5775 (0.1%)
1	C	0.47	0/4232	0.64	3/5760 (0.1%)
1	D	0.47	0/4236	0.61	2/5766 (0.0%)
1	E	0.48	0/4232	0.64	3/5761 (0.1%)
1	F	0.46	0/4244	0.62	2/5776 (0.0%)
All	All	0.48	1/25414 (0.0%)	0.63	14/34592 (0.0%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	CYS	CB-SG	-6.06	1.72	1.82

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	426	THR	C-N-CD	-12.82	92.41	120.60
1	B	426	THR	C-N-CD	-12.28	93.59	120.60
1	F	426	THR	C-N-CD	-11.75	94.75	120.60
1	E	426	THR	C-N-CD	-11.30	95.74	120.60
1	D	426	THR	C-N-CD	-10.62	97.23	120.60
1	A	426	THR	C-N-CD	-10.44	97.63	120.60
1	C	506	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	506	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	163	ASP	CB-CG-OD1	5.89	123.61	118.30
1	D	163	ASP	CB-CG-OD1	5.62	123.36	118.30
1	F	254	LEU	CA-CB-CG	5.61	128.21	115.30
1	E	254	LEU	CA-CB-CG	5.38	127.66	115.30
1	B	163	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	359	ARG	NE-CZ-NH1	5.07	122.84	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	426	THR	Peptide
1	B	426	THR	Peptide
1	C	426	THR	Peptide
1	D	426	THR	Peptide
1	E	426	THR	Peptide
1	F	426	THR	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	4121	0	3912	27	0
1	B	4136	0	3928	27	0
1	C	4122	0	3921	39	0
1	D	4129	0	3919	26	0
1	E	4125	0	3916	22	0
1	F	4134	0	3928	29	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	1	0
2	D	15	0	0	1	0
2	E	45	0	0	3	0
2	F	30	0	0	1	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
3	E	5	0	0	1	0
3	F	15	0	0	0	0
4	A	8	0	14	1	0
4	B	8	0	14	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	B	1	0	0	3	0
6	C	2	0	0	5	0
6	E	1	0	0	3	0
7	A	390	0	0	4	2
7	B	488	0	0	6	2
7	C	424	0	0	4	2
7	D	412	0	0	1	1
7	E	490	0	0	3	4
7	F	436	0	0	3	2
All	All	27633	0	23552	172	7

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 (172) 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:D:345:THR:HG22	1:D:347:ASP:H	1.23	0.99
1:A:232:MET:HE2	1:A:250:PRO:HB2	1.45	0.98
1:A:232:MET:HE3	1:A:252:TYR:HB3	1.44	0.98
1:D:490:MET:HE3	1:D:522:LEU:HB3	1.45	0.97
1:C:345:THR:HG22	1:C:347:ASP:H	1.33	0.92
1:F:334:ASN:HB3	1:F:336:GLN:H	1.43	0.82
1:A:232:MET:HE2	1:A:250:PRO:CB	2.10	0.82
1:A:232:MET:CE	1:A:252:TYR:HB3	2.11	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ALA:HB2	1:E:440:MET:HE3	1.66	0.77
1:C:506:ARG:NH2	7:C:801:HOH:O	2.04	0.76
1:C:584:ARG:NH2	1:C:601:ALA:O	2.18	0.76
1:F:345:THR:HG23	1:F:347:ASP:H	1.49	0.74
4:A:705:MPD:O2	7:A:801:HOH:O	2.01	0.74
1:F:442:LYS:NZ	7:F:802:HOH:O	2.22	0.72
1:B:261:GLY:O	1:B:265:THR:HG23	1.90	0.71
1:A:210:ARG:NH1	7:A:804:HOH:O	2.23	0.71
1:C:334:ASN:O	1:C:336:GLN:N	2.23	0.71
1:C:247:ALA:HB3	1:C:486:LEU:HD23	1.74	0.68
1:B:261:GLY:HA3	6:B:707:CL:CL	2.31	0.68
1:A:232:MET:CE	1:A:250:PRO:HB2	2.23	0.68
1:D:246:VAL:HG23	1:D:544:LEU:HD22	1.75	0.67
1:A:262:ALA:HB2	1:A:440:MET:HE3	1.76	0.66
1:B:48:ARG:NH1	7:B:802:HOH:O	2.28	0.66
1:F:427:PRO:HD3	1:F:456:SER:HB3	1.77	0.65
1:C:309:LEU:HD21	1:C:591:ILE:HD12	1.79	0.65
3:E:704:SO4:O3	7:E:801:HOH:O	2.13	0.65
1:E:246:VAL:HG23	1:E:544:LEU:HD22	1.79	0.64
1:D:262:ALA:HB2	1:D:440:MET:HE3	1.80	0.64
1:A:326:PRO:HB2	1:A:354:VAL:HG13	1.80	0.64
1:A:334:ASN:O	1:A:336:GLN:N	2.30	0.64
1:C:480:ARG:NH1	7:C:803:HOH:O	2.22	0.63
1:A:325:ASP:OD1	1:A:358:LYS:HE2	1.99	0.63
1:A:246:VAL:HG23	1:A:544:LEU:HD22	1.79	0.62
1:B:247:ALA:HB3	1:B:486:LEU:HD23	1.82	0.61
1:D:43:VAL:N	7:D:803:HOH:O	2.31	0.61
1:C:440:MET:HE2	6:C:704:CL:CL	2.38	0.61
1:C:261:GLY:HA3	6:C:704:CL:CL	2.38	0.60
1:C:584:ARG:HG3	1:C:600:ALA:HB3	1.83	0.60
1:F:309:LEU:HD21	1:F:591:ILE:HG23	1.83	0.60
1:F:345:THR:CG2	1:F:347:ASP:H	2.14	0.60
1:A:427:PRO:HD3	1:A:456:SER:CB	2.31	0.60
1:D:528:HIS:HE1	2:D:701:J1K:N1B	1.99	0.59
1:E:309:LEU:HD21	1:E:591:ILE:HG23	1.84	0.59
1:D:427:PRO:HD3	1:D:456:SER:CB	2.31	0.59
1:C:427:PRO:HD3	1:C:456:SER:CB	2.32	0.58
1:D:309:LEU:HD21	1:D:591:ILE:HG23	1.87	0.57
1:F:427:PRO:HD3	1:F:456:SER:CB	2.34	0.56
1:B:265:THR:HG22	7:B:916:HOH:O	2.05	0.56
1:A:247:ALA:HB3	1:A:486:LEU:HD23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:GLY:HA3	6:E:706:CL:CL	2.41	0.56
1:E:427:PRO:HD3	1:E:456:SER:CB	2.35	0.56
1:F:246:VAL:HG23	1:F:544:LEU:HD22	1.88	0.56
1:B:584:ARG:HG3	1:B:600:ALA:HB3	1.88	0.55
1:B:440:MET:HE2	6:B:707:CL:CL	2.44	0.55
1:F:262:ALA:HA	1:F:440:MET:HE3	1.89	0.54
1:C:265:THR:HG22	1:C:441:MET:CE	2.37	0.54
1:C:225:SER:OG	1:C:528:HIS:HE1	1.90	0.54
1:D:60:ASP:OD1	1:D:60:ASP:N	2.39	0.54
1:F:60:ASP:OD1	1:F:60:ASP:N	2.36	0.53
1:C:266:GLN:HA	1:C:441:MET:HE1	1.91	0.53
1:B:262:ALA:CA	1:B:440:MET:HE3	2.39	0.53
1:D:247:ALA:HB3	1:D:486:LEU:HD23	1.90	0.53
1:D:584:ARG:NH1	1:D:601:ALA:O	2.42	0.53
1:B:225:SER:OG	1:B:528:HIS:HE1	1.93	0.52
1:A:427:PRO:HD3	1:A:456:SER:HB3	1.91	0.52
1:C:265:THR:HG22	1:C:441:MET:HE2	1.91	0.52
1:F:247:ALA:HB3	1:F:486:LEU:HD23	1.90	0.51
1:D:56:ASP:HB3	1:D:59:GLY:HA3	1.92	0.51
1:C:440:MET:CE	6:C:704:CL:CL	2.95	0.51
1:B:135:GLY:HA2	1:B:166:HIS:O	2.12	0.50
1:E:427:PRO:HD3	1:E:456:SER:HB3	1.94	0.50
1:F:162:THR:HB	1:F:200:VAL:HG21	1.93	0.50
1:F:306:LEU:O	7:F:801:HOH:O	2.18	0.50
1:C:334:ASN:C	1:C:336:GLN:H	2.14	0.50
1:D:46:ALA:HA	1:D:211:PHE:CZ	2.47	0.50
1:F:262:ALA:CA	1:F:440:MET:HE3	2.42	0.50
1:B:440:MET:CE	6:B:707:CL:CL	2.97	0.49
1:F:225:SER:HG	1:F:528:HIS:CE1	2.30	0.49
1:B:114:ARG:NH1	1:B:137:LEU:HD13	2.27	0.49
3:A:704:SO4:O1	7:A:802:HOH:O	2.19	0.49
1:B:56:ASP:OD2	7:B:801:HOH:O	2.20	0.49
1:E:100:LYS:HD3	1:E:110:GLU:HB3	1.94	0.49
1:A:232:MET:HE2	1:A:250:PRO:CG	2.41	0.49
1:A:225:SER:HA	1:A:249:ALA:O	2.13	0.48
1:D:492:ASP:OD2	1:D:528:HIS:HD2	1.96	0.48
1:E:150:ALA:HB2	2:E:701:J1K:C1	2.42	0.48
1:F:263:TRP:CD2	1:F:364:PRO:HA	2.48	0.48
1:A:209:ALA:HB1	1:F:62:VAL:HG11	1.96	0.48
1:C:64:PRO:HD2	6:C:705:CL:CL	2.50	0.48
1:F:263:TRP:HB2	1:F:364:PRO:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:VAL:HG23	1:C:544:LEU:HD22	1.96	0.47
1:E:263:TRP:CD2	1:E:364:PRO:HA	2.49	0.47
1:B:162:THR:HB	1:B:200:VAL:HG21	1.96	0.47
1:C:46:ALA:HA	1:C:211:PHE:CZ	2.49	0.47
1:B:560:TRP:HB3	1:B:573:THR:HG22	1.97	0.47
1:C:427:PRO:HD3	1:C:456:SER:HB2	1.97	0.47
1:D:135:GLY:HA2	1:D:166:HIS:O	2.14	0.47
1:D:263:TRP:CD2	1:D:364:PRO:HA	2.49	0.47
1:E:214:ARG:NH2	7:E:814:HOH:O	2.47	0.47
1:C:266:GLN:HG2	1:C:441:MET:HE1	1.96	0.47
1:E:162:THR:HB	1:E:200:VAL:HG21	1.97	0.46
1:E:302:THR:HG22	7:E:892:HOH:O	2.16	0.46
1:F:277:ALA:N	7:F:811:HOH:O	2.42	0.46
1:E:150:ALA:HB2	2:E:701:J1K:CA	2.46	0.46
1:F:126:PHE:O	1:F:159:THR:HA	2.16	0.46
1:F:414:GLY:O	1:F:418:ARG:HG3	2.15	0.46
1:C:262:ALA:CA	1:C:440:MET:HE3	2.46	0.46
1:F:331:ASN:HB3	1:F:334:ASN:HB2	1.98	0.46
1:F:432:PRO:HD2	1:F:435:GLN:HG3	1.98	0.46
1:B:263:TRP:CD2	1:B:364:PRO:HA	2.51	0.45
1:D:56:ASP:CB	1:D:59:GLY:HA3	2.45	0.45
1:D:383:SER:OG	1:D:384:GLY:N	2.48	0.45
1:E:492:ASP:OD2	1:E:528:HIS:HD2	1.98	0.45
1:C:263:TRP:CD2	1:C:364:PRO:HA	2.51	0.45
1:C:345:THR:HB	1:C:348:CYS:HB2	1.99	0.45
1:E:528:HIS:HE1	2:E:703:J1K:N1B	2.15	0.45
1:C:266:GLN:HA	1:C:441:MET:CE	2.46	0.45
1:C:100:LYS:HG3	7:C:927:HOH:O	2.16	0.45
1:D:427:PRO:HD3	1:D:456:SER:HB3	1.98	0.44
1:B:302:THR:HG22	7:B:861:HOH:O	2.17	0.44
1:C:97:ALA:HB3	1:C:100:LYS:HZ3	1.82	0.44
1:A:263:TRP:CD2	1:A:364:PRO:HA	2.53	0.44
1:B:399:LEU:C	1:B:409:ALA:HB2	2.38	0.44
1:D:108:PRO:HG2	1:D:170:VAL:HG11	1.99	0.44
1:A:46:ALA:HA	1:A:211:PHE:CZ	2.52	0.44
1:C:410:GLN:OE1	7:C:802:HOH:O	2.21	0.43
1:D:345:THR:HG22	1:D:347:ASP:N	2.08	0.43
1:D:263:TRP:HB2	1:D:364:PRO:HB3	1.99	0.43
1:F:225:SER:OG	2:F:701:J1K:CB	2.67	0.43
1:B:262:ALA:HA	1:B:440:MET:HE3	2.00	0.43
1:D:43:VAL:HA	1:D:44:PRO:HD3	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:HG23	1:B:544:LEU:HD22	1.99	0.43
1:C:177:LEU:HD12	1:C:422:VAL:HG23	2.01	0.43
1:A:294:LEU:HD11	1:A:348:CYS:N	2.34	0.43
1:C:263:TRP:HB2	1:C:364:PRO:HB3	2.00	0.43
1:A:56:ASP:O	7:A:803:HOH:O	2.21	0.43
1:B:309:LEU:HD11	1:B:591:ILE:CD1	2.49	0.42
1:C:164:GLY:HA2	1:C:196:SER:OG	2.19	0.42
1:B:225:SER:OG	1:B:528:HIS:CE1	2.73	0.42
1:D:427:PRO:HA	1:D:428:PRO:HD2	1.90	0.42
1:E:141:THR:O	1:E:151:SER:HB2	2.20	0.42
1:B:341:VAL:N	7:B:817:HOH:O	2.52	0.42
1:A:100:LYS:HG2	1:A:110:GLU:OE2	2.20	0.42
1:E:135:GLY:HA2	1:E:166:HIS:O	2.19	0.42
1:F:427:PRO:HA	1:F:428:PRO:HD2	1.90	0.42
1:C:354:VAL:O	1:C:358:LYS:HG3	2.19	0.42
1:A:225:SER:HG	1:A:528:HIS:CE1	2.37	0.42
1:A:401:SER:H	1:A:408:ASN:HD21	1.68	0.42
1:C:135:GLY:HA2	1:C:166:HIS:O	2.20	0.41
1:E:440:MET:CE	6:E:706:CL:CL	3.05	0.41
1:A:248:GLY:HA3	1:A:487:TYR:CZ	2.56	0.41
1:C:222:ILE:HG12	1:C:246:VAL:HB	2.01	0.41
1:F:251:GLY:O	1:F:254:LEU:HB2	2.19	0.41
1:B:528:HIS:CE1	7:B:899:HOH:O	2.74	0.41
1:F:254:LEU:HD13	1:F:495:PHE:CE1	2.56	0.41
1:B:309:LEU:HD11	1:B:591:ILE:HD11	2.03	0.41
1:C:258:GLY:HA2	6:C:704:CL:CL	2.58	0.41
1:E:225:SER:HA	1:E:249:ALA:O	2.20	0.41
1:B:100:LYS:HG2	1:B:110:GLU:OE2	2.20	0.41
1:E:210:ARG:HE	1:E:210:ARG:HB2	1.48	0.41
1:F:141:THR:O	1:F:151:SER:HB2	2.21	0.41
1:C:225:SER:OG	1:C:528:HIS:CE1	2.73	0.41
1:D:490:MET:CE	1:D:522:LEU:HD22	2.51	0.41
1:E:177:LEU:HD12	1:E:422:VAL:HG23	2.02	0.41
1:E:440:MET:HE1	6:E:706:CL:CL	2.58	0.41
1:A:427:PRO:HA	1:A:428:PRO:HD2	1.88	0.41
1:C:210:ARG:HB2	2:C:701:J1K:O9	2.21	0.40
1:A:243:ASP:O	1:A:482:GLY:HA2	2.22	0.40
1:B:222:ILE:HG12	1:B:246:VAL:HB	2.03	0.40
1:D:462:SER:O	1:D:465:ASP:HB2	2.22	0.40
3:B:703:SO4:O4	1:C:199:GLN:NE2	2.53	0.40
1:F:225:SER:HA	1:F:249:ALA:O	2.21	0.40

All (7) 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)
7:A:1171:HOH:O	7:E:1063:HOH:O[4_545]	2.00	0.20
7:D:1202:HOH:O	7:E:1252:HOH:O[2_554]	2.09	0.11
7:B:1273:HOH:O	7:E:1196:HOH:O[4_445]	2.12	0.08
7:C:1191:HOH:O	7:F:1187:HOH:O[2_455]	2.12	0.08
7:C:1220:HOH:O	7:F:1105:HOH:O[2_455]	2.12	0.08
7:B:1094:HOH:O	7:B:1218:HOH:O[4_545]	2.14	0.06
7:A:1013:HOH:O	7:E:1086:HOH:O[4_545]	2.18	0.02

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	554/596 (93%)	536 (97%)	16 (3%)	2 (0%)	34	32
1	B	555/596 (93%)	538 (97%)	16 (3%)	1 (0%)	47	49
1	C	554/596 (93%)	534 (96%)	18 (3%)	2 (0%)	34	32
1	D	555/596 (93%)	541 (98%)	13 (2%)	1 (0%)	47	49
1	E	554/596 (93%)	537 (97%)	15 (3%)	2 (0%)	34	32
1	F	556/596 (93%)	536 (96%)	18 (3%)	2 (0%)	34	32
All	All	3328/3576 (93%)	3222 (97%)	96 (3%)	10 (0%)	41	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	PRO
1	B	427	PRO
1	C	427	PRO
1	D	427	PRO
1	E	427	PRO
1	F	427	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	335	GLY
1	E	225	SER
1	A	335	GLY
1	F	225	SER

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	405/439 (92%)	393 (97%)	12 (3%)	41	44
1	B	407/439 (93%)	394 (97%)	13 (3%)	39	41
1	C	406/439 (92%)	400 (98%)	6 (2%)	65	71
1	D	406/439 (92%)	397 (98%)	9 (2%)	52	57
1	E	406/439 (92%)	398 (98%)	8 (2%)	55	60
1	F	407/439 (93%)	396 (97%)	11 (3%)	44	48
All	All	2437/2634 (92%)	2378 (98%)	59 (2%)	49	53

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	241	HIS
1	A	254	LEU
1	A	278	GLN
1	A	294	LEU
1	A	358	LYS
1	A	375	ARG
1	A	405	SER
1	A	467	HIS
1	A	538	PHE
1	A	591	ILE
1	A	594	GLU
1	B	43	VAL
1	B	71	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	137	LEU
1	B	190	LEU
1	B	241	HIS
1	B	254	LEU
1	B	265	THR
1	B	278	GLN
1	B	302	THR
1	B	338	LEU
1	B	352	VAL
1	B	375	ARG
1	B	467	HIS
1	C	43	VAL
1	C	241	HIS
1	C	254	LEU
1	C	278	GLN
1	C	338	LEU
1	C	375	ARG
1	D	102	THR
1	D	210	ARG
1	D	241	HIS
1	D	254	LEU
1	D	278	GLN
1	D	285	LYS
1	D	338	LEU
1	D	375	ARG
1	D	401	SER
1	E	137	LEU
1	E	179	THR
1	E	190	LEU
1	E	241	HIS
1	E	254	LEU
1	E	302	THR
1	E	338	LEU
1	E	375	ARG
1	F	70	VAL
1	F	137	LEU
1	F	214	ARG
1	F	241	HIS
1	F	254	LEU
1	F	278	GLN
1	F	302	THR
1	F	338	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	345	THR
1	F	375	ARG
1	F	467	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	528	HIS
1	C	528	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 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	SO4	F	705	-	4,4,4	0.15	0	6,6,6	0.12	0
2	J1K	C	702	-	15,15,15	0.71	1 (6%)	19,19,19	1.40	3 (15%)
3	SO4	E	704	-	4,4,4	0.18	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	J1K	F	702	-	15,15,15	0.63	0	19,19,19	1.09	1 (5%)
2	J1K	C	701	-	15,15,15	0.56	0	19,19,19	1.33	2 (10%)
2	J1K	E	701	-	15,15,15	0.88	0	19,19,19	0.96	0
2	J1K	E	703	-	15,15,15	0.73	0	19,19,19	1.22	2 (10%)
3	SO4	B	703	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	A	702	-	4,4,4	0.20	0	6,6,6	0.15	0
2	J1K	B	701	-	15,15,15	0.80	1 (6%)	19,19,19	1.36	2 (10%)
3	SO4	F	704	-	4,4,4	0.18	0	6,6,6	0.13	0
2	J1K	D	701	-	15,15,15	0.73	0	19,19,19	1.21	1 (5%)
4	MPD	B	705	-	7,7,7	0.37	0	9,10,10	0.68	0
3	SO4	A	704	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	B	702	-	4,4,4	0.17	0	6,6,6	0.11	0
2	J1K	F	701	-	15,15,15	0.80	1 (6%)	19,19,19	0.86	0
4	MPD	A	705	-	7,7,7	0.26	0	9,10,10	0.59	0
2	J1K	E	702	-	15,15,15	0.60	0	19,19,19	0.58	0
3	SO4	A	703	-	4,4,4	0.17	0	6,6,6	0.17	0
3	SO4	B	704	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	F	703	-	4,4,4	0.16	0	6,6,6	0.18	0
2	J1K	A	701	-	15,15,15	0.78	1 (6%)	19,19,19	1.05	0

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	J1K	E	701	-	-	0/12/12/12	0/1/1/1
2	J1K	C	702	-	-	3/12/12/12	0/1/1/1
2	J1K	F	701	-	-	3/12/12/12	0/1/1/1
4	MPD	A	705	-	-	1/5/5/5	-
2	J1K	E	702	-	-	0/12/12/12	0/1/1/1
2	J1K	F	702	-	-	2/12/12/12	0/1/1/1
2	J1K	E	703	-	-	1/12/12/12	0/1/1/1
2	J1K	B	701	-	-	3/12/12/12	0/1/1/1
2	J1K	A	701	-	-	1/12/12/12	0/1/1/1
2	J1K	D	701	-	-	3/12/12/12	0/1/1/1
2	J1K	C	701	-	-	3/12/12/12	0/1/1/1
4	MPD	B	705	-	-	4/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	J1K	O2A-CA	-2.44	1.23	1.30
2	A	701	J1K	O2A-CA	-2.31	1.23	1.30
2	C	702	J1K	O2A-CA	-2.21	1.23	1.30
2	F	701	J1K	O2A-CA	-2.04	1.24	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	702	J1K	O2B-CB-C4	2.97	126.23	120.94
2	E	703	J1K	O2B-CB-C4	2.88	126.07	120.94
2	B	701	J1K	C7-N1B-CB	-2.65	116.05	122.08
2	E	703	J1K	C7-N1B-CB	-2.56	116.25	122.08
2	B	701	J1K	O2B-CB-C4	2.54	125.47	120.94
2	D	701	J1K	O2B-CB-C4	2.40	125.21	120.94
2	C	702	J1K	C7-N1B-CB	-2.35	116.72	122.08
2	C	701	J1K	O1A-CA-C1	-2.29	115.34	121.45
2	C	701	J1K	C6-C1-C2	2.25	121.79	118.59
2	C	702	J1K	O2A-CA-C1	2.13	120.37	114.85
2	F	702	J1K	C2-C1-CA	-2.07	116.31	120.39

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	J1K	N1B-C7-C8-O9
2	B	701	J1K	N1B-C7-C8-O9
2	C	701	J1K	C4-CB-N1B-C7
2	C	702	J1K	C4-CB-N1B-C7
2	C	702	J1K	N1B-C7-C8-O9
2	D	701	J1K	C4-CB-N1B-C7
2	E	703	J1K	N1B-C7-C8-O9
2	F	701	J1K	C4-CB-N1B-C7
2	F	702	J1K	C4-CB-N1B-C7
4	B	705	MPD	C1-C2-C3-C4
2	C	701	J1K	O2B-CB-N1B-C7
2	F	701	J1K	O2B-CB-N1B-C7
2	F	702	J1K	O2B-CB-N1B-C7
2	B	701	J1K	C4-CB-N1B-C7
2	D	701	J1K	O2B-CB-N1B-C7
2	C	702	J1K	O2B-CB-N1B-C7
2	C	701	J1K	N1B-C7-C8-O9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	701	J1K	O2B-CB-N1B-C7
2	F	701	J1K	N1B-C7-C8-O9
2	D	701	J1K	N1B-C7-C8-O9
4	B	705	MPD	O2-C2-C3-C4
4	B	705	MPD	CM-C2-C3-C4
4	A	705	MPD	C2-C3-C4-O4
4	B	705	MPD	C2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	704	SO4	1	0
2	C	701	J1K	1	0
2	E	701	J1K	2	0
2	E	703	J1K	1	0
3	B	703	SO4	1	0
2	D	701	J1K	1	0
3	A	704	SO4	1	0
2	F	701	J1K	1	0
4	A	705	MPD	1	0

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	558/596 (93%)	0.06	32 (5%)	23	29	20, 29, 51, 76	0
1	B	558/596 (93%)	-0.27	9 (1%)	72	75	18, 24, 36, 84	0
1	C	557/596 (93%)	-0.17	7 (1%)	77	80	19, 27, 44, 62	0
1	D	559/596 (93%)	-0.15	16 (2%)	51	57	19, 27, 44, 76	0
1	E	558/596 (93%)	-0.11	11 (1%)	65	69	18, 24, 38, 93	0
1	F	559/596 (93%)	-0.21	7 (1%)	77	80	20, 27, 42, 78	0
All	All	3349/3576 (93%)	-0.14	82 (2%)	59	64	18, 26, 44, 93	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ASP	5.6
1	D	341	VAL	5.2
1	E	56	ASP	4.7
1	F	43	VAL	4.6
1	A	341	VAL	4.5
1	A	43	VAL	4.4
1	A	59	GLY	4.2
1	E	343	ALA	4.2
1	A	345	THR	3.9
1	E	603	PRO	3.9
1	D	43	VAL	3.9
1	A	346	ALA	3.8
1	F	56	ASP	3.7
1	F	44	PRO	3.6
1	A	602	PRO	3.6
1	D	59	GLY	3.6
1	A	403	ASN	3.5
1	B	43	VAL	3.4
1	D	343	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	603	PRO	3.3
1	E	341	VAL	3.3
1	D	44	PRO	3.3
1	B	56	ASP	3.2
1	F	368	ALA	3.2
1	A	340	CYS	3.1
1	F	603	PRO	3.0
1	B	388	THR	3.0
1	A	333	ALA	3.0
1	A	369	GLY	2.9
1	F	341	VAL	2.9
1	D	333	ALA	2.9
1	A	405	SER	2.9
1	A	48	ARG	2.9
1	A	402	PHE	2.8
1	A	60	ASP	2.8
1	A	388	THR	2.7
1	D	603	PRO	2.6
1	A	601	ALA	2.5
1	D	345	THR	2.5
1	E	43	VAL	2.5
1	E	602	PRO	2.4
1	A	273	VAL	2.4
1	A	343	ALA	2.4
1	B	403	ASN	2.4
1	A	334	ASN	2.4
1	D	48	ARG	2.4
1	A	387	GLY	2.4
1	B	603	PRO	2.4
1	B	48	ARG	2.4
1	E	60	ASP	2.3
1	A	368	ALA	2.3
1	A	437	ALA	2.3
1	C	43	VAL	2.3
1	C	346	ALA	2.3
1	D	369	GLY	2.3
1	D	368	ALA	2.3
1	A	389	THR	2.3
1	C	587	GLY	2.3
1	E	368	ALA	2.2
1	E	388	THR	2.2
1	A	234	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	277	ALA	2.2
1	D	56	ASP	2.2
1	A	370	THR	2.2
1	A	348	CYS	2.2
1	D	60	ASP	2.2
1	B	387	GLY	2.2
1	A	390	TYR	2.1
1	C	367	SER	2.1
1	D	52	GLU	2.1
1	B	60	ASP	2.1
1	B	341	VAL	2.1
1	C	238	PHE	2.1
1	C	403	ASN	2.1
1	F	60	ASP	2.1
1	D	336	GLN	2.1
1	A	434	THR	2.1
1	E	234	LEU	2.0
1	A	238	PHE	2.0
1	D	335	GLY	2.0
1	A	433	MET	2.0
1	E	231	GLY	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 monosaccharides 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. 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	J1K	E	701	15/15	0.74	0.21	34,48,59,61	0
4	MPD	A	705	8/8	0.78	0.28	54,62,64,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	J1K	F	702	15/15	0.80	0.21	54,55,61,62	0
2	J1K	C	701	15/15	0.81	0.19	40,48,63,64	0
3	SO4	F	705	5/5	0.85	0.20	110,111,113,114	0
2	J1K	E	702	15/15	0.86	0.14	44,46,55,60	0
3	SO4	F	704	5/5	0.86	0.31	102,103,106,108	0
3	SO4	B	704	5/5	0.90	0.12	78,82,85,86	0
3	SO4	A	704	5/5	0.91	0.23	100,100,105,106	0
3	SO4	B	702	5/5	0.91	0.31	102,102,107,109	0
3	SO4	A	703	5/5	0.91	0.20	92,93,97,97	0
3	SO4	E	704	5/5	0.92	0.23	97,98,99,103	0
3	SO4	A	702	5/5	0.92	0.14	75,77,78,79	0
3	SO4	F	703	5/5	0.93	0.13	85,86,86,88	0
3	SO4	B	703	5/5	0.93	0.18	90,92,96,98	0
2	J1K	C	702	15/15	0.95	0.11	16,21,51,56	0
2	J1K	D	701	15/15	0.95	0.11	19,24,38,44	0
4	MPD	B	705	8/8	0.95	0.14	26,31,36,37	0
2	J1K	A	701	15/15	0.96	0.11	23,25,51,59	0
2	J1K	B	701	15/15	0.96	0.10	12,17,42,51	0
6	CL	B	707	1/1	0.96	0.17	61,61,61,61	0
2	J1K	E	703	15/15	0.97	0.14	15,20,46,50	0
2	J1K	F	701	15/15	0.97	0.10	17,21,39,45	0
6	CL	C	704	1/1	0.97	0.16	58,58,58,58	0
6	CL	C	705	1/1	0.97	0.20	66,66,66,66	0
6	CL	E	706	1/1	0.97	0.09	51,51,51,51	0
5	CA	C	703	1/1	0.98	0.03	30,30,30,30	0
5	CA	A	706	1/1	0.99	0.04	25,25,25,25	0
5	CA	D	702	1/1	0.99	0.03	21,21,21,21	0
5	CA	E	705	1/1	0.99	0.05	26,26,26,26	0
5	CA	F	706	1/1	0.99	0.04	24,24,24,24	0
5	CA	B	706	1/1	1.00	0.03	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.